Post-Newtonian Description of Quantum Systems in Gravitational Fields

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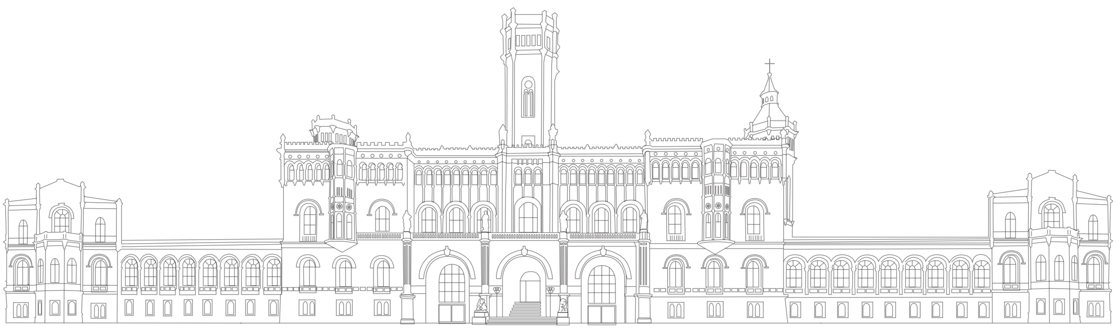

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Abstract

This thesis deals with the systematic treatment of quantum-mechanical systems situated in post-Newtonian gravitational fields. At first, we develop a framework of geometric background structures that define the notions of a post-Newtonian expansion and of weak gravitational fields. Next, we consider the description of single quantum particles under gravity, before continuing with a simple composite system. Starting from clearly spelled-out assumptions, our systematic approach allows to properly *derive* the post-Newtonian coupling of quantum-mechanical systems to gravity based on first principles. This sets it apart from other, more heuristic approaches that are commonly employed, for example, in the description of quantum-optical experiments under gravitational influence.

Regarding single particles, we compare simple canonical quantisation of a free particle in curved spacetime to formal expansions of the minimally coupled Klein–Gordon equation, which may be motivated from the framework of quantum field theory in curved spacetimes. Specifically, we develop a general WKB-like post-Newtonian expansion of the Klein–Gordon equation to arbitrary order in the inverse of the velocity of light. Furthermore, for stationary spacetimes, we show that the Hamiltonians arising from expansions of the Klein–Gordon equation and from canonical quantisation agree up to linear order in particle momentum, independent of any expansion in the inverse of the velocity of light.

Concerning the topic of composite systems, we perform a fully detailed systematic derivation of the first order post-Newtonian quantum Hamiltonian describing the dynamics of an electromagnetically bound two-particle system which is situated in external electromagnetic and gravitational fields. This calculation is based on previous work by Sonnleitner and Barnett, which we significantly extend by the inclusion of a weak gravitational field as described by the Eddington–Robertson parametrised post-Newtonian metric.

In the last, independent part of the thesis, we prove two uniqueness results characterising the Newton–Wigner position observable for Poincaré-invariant *classical* Hamiltonian systems: one is a direct classical analogue of the well-known quantum Newton–Wigner theorem, and the other clarifies the geometric interpretation of the Newton–Wigner position as 'centre of spin', as proposed by Fleming in 1965.

Keywords: quantum systems under gravity, post-Newtonian expansion, post-Newtonian gravity, weak gravity

Zusammenfassung

Diese Arbeit beschäftigt sich mit der systematischen Beschreibung quantenmechanischer Systeme in post-Newton'schen Gravitationsfeldern. Zunächst entwickeln wir geometrische Hintergrundstrukturen, welche die Konzepte einer post-Newton'schen Entwicklung und schwacher Gravitationsfelder zu definieren ermöglichen. Anschließend beschäftigen wir uns mit der Beschreibung einzelner Quantenteilchen unter Gravitation und wenden uns schließlich einem einfachen zusammengesetzten System zu. Unsere von klar formulierten Annahmen ausgehende systematische Vorgehensweise ermöglicht es, die post-Newton'sche Kopplung quantenmechanischer Systeme an Gravitation im eigentlichen Sinne *herzuleiten*. Dies unterscheidet sie von anderen, heuristischeren Herangehensweisen, wie sie beispielsweise oft zur Beschreibung quantenoptischer Experimente unter Gravitation benutzt werden.

Für einzelne Teilchen vergleichen wir die einfache kanonische Quantisierung freier Teilchen in gekrümmten Raumzeiten mit formalen Entwicklungen der minimal gekoppelten Klein-Gordon-Gleichung, welche quantenfeldtheoretisch motiviert werden können. Konkret entwickeln wir eine allgemeine WKB-artige post-Newton'sche Entwicklung der Klein-Gordon-Gleichung zu beliebiger Ordnung im Inversen der Lichtgeschwindigkeit. Ferner zeigen wir für stationäre Raumzeiten, dass die Hamilton-Operatoren, welche aus Entwicklungen der Klein-Gordon-Gleichung bzw. mit kanonischer Quantisierung hergeleitet werden, zu linearer Ordnung im Teilchenimpuls übereinstimmen, unabhängig von jeglicher Entwicklung im Inversen der Lichtgeschwindigkeit.

Wir leiten den in erster Ordnung post-Newton'schen Hamiltonoperator vollständig her, der die Dynamik eines elektromagnetisch gebundenen Zwei-Teilchen-Systems beschreibt, das sich in sowohl einem externen elektromagnetischen als auch einem Gravitationsfeld befindet. Diese Rechnung basiert auf einer Arbeit von Sonnleitner und Barnett, die wir durch die Einbeziehung der Gravitation maßgeblich erweitern.

Im letzten, unabhängigen Teil der Arbeit beweisen wir zwei Eindeutigkeitsresultate über die Newton-Wigner-Ortsobservable für Poincaré-invariante *klassische* Hamilton'sche Systeme. Eines ist ein direktes klassisches Analogon des quantenmechanischen Newton-Wigner-Satzes; das andere gibt eine klare Charakterisierung der geometrischen Interpretation des Newton-Wigner-Orts als „Spin-Zentrum", die 1965 von Fleming vorgeschlagen wurde.

Schlagworte: Quantensysteme unter Gravitation, post-Newton'sche Entwicklung, post-Newton'sche Gravitation, schwache Gravitation

Summarium[1]

hoc opus est de descriptione sastematica systematium mechanicorum quanticorum in campis gravitalibus post Newtonum. primo recessas structuras geometricas elaborabimus, quibus consilia expansionis post Newtonum parvisque campis gravitalibus definiri potest. deinde descriptioni singulorum particulorum quanticorum sub gravitatione studebimus atque ultimo in systemate composito facili versabimur. ab praesumptionibus clare conceptis systematice procedenti post Newtonum copulationem systematium mechanicorum quanticorum ad gravitationem proprie *dedicare* poterimus. qui modus procedendi ab aliis, heuristicis, velut ad experimenta optica quantica describendum utuntur, differt.

quod attinet ad singula particula, quantificationem canonicam facilem particulorum nullas vires experientum in spatiotemporibus curvatis cum expansionibus formalibus equationis Kleini Gordonique minime copulatae, quae ex ratione quanticorum camporum motivari possunt, comparabimus. proprie ad dicendum post Newtonum expansionem generalem WKB-bilem equitationis Kleini Gordonique ad quamlibet ordinem in inverso velocitatis lucis faciemus. quod praeterea attinet ad spatiotempora stationaria, operatores Hamiltoni de expansionibus equationis Kleini Gordonique aut cum quantificatione canonica dedicatos in ordine lineali inter se impetu particulorum consentire demonstrabimus. quod non obnoxium cuicumque expansioni in inverso velocitatis lucis est.

quod attinet ad systemata coniuncta, operatorem Hamiltoni in prima ordine post Newtonum radicite dedicemus, qui dynamiken systematis ex duobus particulis electromagnetice coniuncti describit, quod et in campo electromagnetico et in campo gravitale est. quae ratio in opere Sonnleitneri Barnettique posita est, quod gravitationem comprehendendo augebimus multo.

ultima in parte absoluta huius operis duos exitus perspicuitatis de loci quantitate Newtoni Wignerique, quod attinet ad systemata Hamiltoni classica invarianta secundum Poincareum, demonstrabimus. alius est analogon classicum directum mechanici quantici theorematis Newtoni Wignerique; alio locus Newtoni Wignerique pro 'medio impetus rotationis interni' geometrice interpretatur, ut Flemingus proposit anno MMDCCXVIII ab urbe condita.

proposita: systemata quantica in gravitatione, expansio post Newtonum, gravitatio post Newtonum, gravitatio parva

[1]translatus de Philippo Sandero

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Contents

1. Introduction

Imagine we are given a quantum-mechanical system whose time evolution in the absence of gravity is known in terms of the ordinary time-dependent Schrödinger equation. In other words: we know the system's Hamiltonian if all gravitational interactions are neglected. We now ask: which principles do we use in order to deduce the system's interaction with a given external gravitational field? Note that by 'gravitational field' we understand all the ten independent components $g_{\mu\nu}$ of the spacetime metric, subject to Einstein's field equations of general relativity – or, more generally, to the equations of some other metric theory of gravity – and not just the scalar component ϕ representing the Newtonian potential.

In fact, for Newtonian gravity there is no problem at all in describing its coupling to ordinary quantum mechanics: we may simply include a background Newtonian gravitational potential ϕ into the Schrödinger equation describing a 'non-relativistic'[1] particle of mass m and zero spin, giving

$$\mathrm{i}\hbar\partial_t\psi = \left(-\frac{\hbar^2}{2m}\Delta + m\phi\right)\psi. \tag{1.0.1}$$

This equation has extensively been tested in the gravitational field of the earth, beginning with neutron interferometry in the classic Colella–Overhauser–Werner experiment [COW75] and leading up to atom interferometers of the Kasevich–Chu type, accomplishing, e.g., highly precise measurements of the gravitational acceleration g on the earth [Far+14]. We ask what kind of 'post-Newtonian corrections' to this equation arise from general relativity or other metric theories of gravity, considering additional terms involving the Newtonian potential ϕ as well as new terms involving all metric components.

[1] As a matter of principle, we try to avoid the common but misleading adjective 'non-relativistic' to distinguish Galilei-invariant dynamical laws from 'relativistic' ones, by which one then means those obeying Poincaré invariance. It is not the validity of the relativity principle that distinguishes both cases, but rather the way which that principle is implemented in. Nevertheless, since we cannot entirely escape traditionally established nomenclature, we will occasionally use the term 'non-relativistic' in the sense just explained and think of it as always being put between inverted commas.

The behaviour of quantum systems in general gravitational fields is naturally of fundamental conceptual theoretic interest. However, it is also of immediate practical importance, relating to recent experimental developments in quantum optics and matter-wave interferometry: these have now reached a degree of precision that covers 'relativistic corrections' which were hitherto not considered in such settings. In particular, this includes couplings between 'internal' and 'centre of mass' degrees of freedom of composite systems without a Newtonian analogue – as for example induced by post-Newtonian gravitational fields. The most famous example for a possible implication of such couplings is probably the controversially discussed topic of gravitationally induced quantum dephasing [Zyc+11; Pik+15; BOS15; PCK16]. Other experimentally inclined topics for which the gravity–quantum matter coupling beyond Newton is relevant include, for example, atom interferometric gravitational wave detection [GWZ18], quantum tests of the classical equivalence principle [Sch+14], or proposals of quantum formulations of the equivalence principle [ZB18] and tests thereof [Ros+17].

Clearly, such experiments require proper 'relativistic' treatments for their theoretical descriptions, that may be trusted as describing the situation in a correct way. However, the descriptions one finds in the literature are often restricted to the more or less *ad hoc* addition of 'relativistic effects' known from classical physics, such as velocity-dependent masses, second-order Doppler shifts, or redshifted energies and time dilations due to relative velocities and/or gravitational potentials; see, e.g., [Dim+08; Zyc+11; Pik+15; Rou18; Gie+19; Lor+19; ZRP19]. Such approaches are conceptually dangerous for a number of reasons: they neither guarantee completeness and independence of the 'relativistic effects', nor do they need to apply in non-classical situations where quantum properties dominate the dynamics. Namely, as is common in atom interferometry, these treatments make use in an essential way of semi-classical notions like 'wordline' and 'redshift', which have no immediate meaning in quantum theory unless the state of the system is severely restricted in an *a priori* fashion: the overall pure state of the system has to be assumed to separate into the tensor product of a pure state for the centre of mass degrees of freedom with a pure state for the relative degrees of freedom; and furthermore, the state for the centre of mass has to be of semiclassical nature, so as to determine a worldline for which the notion of proper time can be defined.[2] It may well be that these *a priori* restrictions can be justified in specific applications within quantum optics and atom interferometry. However, we wish to promote the view that the theoretical problem of describing the coupling between quantum-mechanical systems and post-Newtonian gravity should be solved *independently* of such restrictions, in a systematic and well-defined way. Such a proper systematic *derivation* of the

[2]We recall that the path integral in ordinary quantum mechanics generally receives contributions from continuous but nowhere differentiable paths. Only in very special situations is the dominant contribution given by the action along a smooth classical path, such that one may define an arc length, i.e. a proper time.

coupling will also make sure that all relevant 'relativistic corrections' to the Newtonian description are present, and that none is included multiple times.

In answering the question of what such a systematic coupling procedure could look like, we have to address a conceptual difficulty that does not arise for classical systems. Namely, for classical matter obeying Poincaré-invariant dynamical laws, there is a systematic, almost algorithmic procedure one can employ in order to couple it to metric theories of gravity: the usual 'minimal coupling scheme'. We recall that, in a nutshell, this scheme consists in a two-step process [MTW73]: first, write down the matter's dynamical law in a Poincaré-invariant fashion in Minkowski spacetime; second, replace the flat Minkowski metric η by the potentially curved Lorentzian metric g of spacetime, and the partial derivatives with respect to the affine inertial coordinates of Minkowski spacetime (i.e. the covariant derivatives with respect to η) by Levi–Civita covariant derivatives with respect to g. This gives a unique way of coupling classical matter fields to metric theories of gravity, up to the well-known issue of curvature ambiguities (arising from the non-commutativity of covariant derivatives in the curved case) and the possibility of non-minimal coupling (i.e. explicit coupling to the curvature tensor).

The minimal coupling scheme is rooted in Einstein's equivalence principle, whose essence is that 'gravity' can be fully encoded in the metric geometry of spacetime, which is *common to all matter components*. We stress that this is the important point, encoding the *universality* of gravitational interaction: any matter component, be it some elementary particle with or without mass, spin, electric charge, or other features, or be it a macroscopic body, like a football or a planet, will couple to gravity in a way that only depends on one and the same geometry of spacetime; compare [TLL73] and [Wil93]. Note that this does in no way imply that all bodies 'fall' in the same way: for a realistic body, which is spinning and/or possesses mass multipoles of higher order than the single monopole of an idealised 'test particle', any approximate 'central worldline' will depend on the characteristics of the body and deviate from that of a test particle (i.e. a geodesic). However, as long as all these deviations find their explanations in couplings to the spacetime geometry, no violation of the equivalence principle should be concluded. This remark also applies in connection with attempts to formulate the equivalence principle in quantum mechanics: simple quantum translations of some notion of 'universality of free fall' – as the Newtonian one proposed in [ZB18] – should not be seen as capturing any core statement of the equivalence principle; to the contrary, they even bear the danger of falsely concluding violations. Furthermore, such formulations depend on notions of 'worldlines', and thus are based on *a priori* assumptions concerning the state of the matter. We are convinced that any possible generally valid implementation of the equivalence principle into quantum mechanics should not make such assumptions. An extensive discussion of these important conceptual issues may be found in our article [SG19b].

We now return to the more concrete question of systematic coupling procedures of quantum mechanics to gravitational fields. The above-mentioned conceptual problem which we face here is that the minimal coupling scheme simply cannot be applied in that case: ordinary quantum mechanics is Galilei-invariant, and so even the first step of the minimal coupling procedure cannot be implemented. As is well-known, enforcing Poincaré symmetry upon quantum mechanics eventually leads to the framework of Poincaré-invariant quantum field theory, often called 'Relativistic Quantum Field Theory' (RQFT), whose mathematical structure and physical interpretation is far more complex than that of ordinary 'non-relativistic' quantum mechanics. In particular, RQFT does not have a form similar to a usual, classical field theory on Minkowski spacetime – i.e. also RQFT cannot be coupled to metric gravity by a direct application of the minimal coupling scheme. Instead, the framework of quantum field theory in curved spacetimes (QFTCS) applies minimal coupling at the *classical* level, and then employs methods to quantise the minimally coupled classical field theories [BF09; Wal94].

So we are lead to accept the fact that it does not seem to be possible to couple an 'already quantised' theory to gravity, and thus to turn to QFTCS as the best available solution for the systematic description of gravity–quantum matter coupling. Does that mean we would have to employ the whole machinery of QFTCS in order to just answer simple questions concerning matter–gravity interactions that go beyond the simplest couplings to the Newtonian potential? We think that the answer is no, at least as long as we are merely interested in leading order 'relativistic corrections' below the threshold of quantum-field-theoretic pair production, and as long as the spacetime geometry is at least approximately stationary, such that there is a consistent field-theoretic concept of particles. At the same time, we think that the alternative to full QFTCS should not consist of *ad hoc* procedures guided by more or less well founded 'physical intuition'. Rather we should look for general and systematic methods that allow to derive the full coupling, and arguably qualify as a proper post-Newtonian approximation. This thesis aims to provide a positive contribution to this end.

1.1. Plan of this thesis

In chapter 2, we will set up the conceptual framework for our systematic post-Newtonian expansions in the following chapters: we introduce a set of geometric background structures that enable us to define the notions of weak gravitational fields and post-Newtonian expansions.

Based on this framework, chapter 3 will deal with the systematic description of *single* quantum particles under gravity. We introduce a simple method of canonical quantisation of a free particle in a post-Newtonian spacetime, and aim to compare its results to methods which are more firmly rooted in first principles. Therefore, motivated from QFTCS, we develop two different kinds of formal post-Newtonian expansions of the minimally coupled Klein–Gordon equation, and compare their results to those from the canonical quantisation method. This will lead to the conclusion that at the lowest relevant post-Newtonian orders, simple canonical quantisation may safely be employed.

Chapter 4 will continue the investigation with the study of a simple *composite* quantum system in post-Newtonian gravity. We consider a simple 'atomic' system consisting of two electromagnetically bound bosonic particles, situated in an external electromagnetic field as well as an external gravitational field described by the Eddington–Robertson parametrised post-Newtonian metric. We give a fully detailed systematic derivation of the first order post-Newtonian quantum Hamiltonian describing the dynamics of the atomic system in this situation.

The last proper chapter 5 is entirely independent of the rest of the thesis: it is concerned with the investigation of the special-relativistic localisation problem for classical (i.e. non-quantum) systems, in particular with characterisations of the Newton–Wigner position observable for such systems. Even though this topic is almost completely disconnected from the description of quantum systems in post-Newtonian gravity, it arose in a natural way from the investigations in chapter 4. For this reason, and due to the particular conceptional and mathematical beauty I (the author) see in the results obtained in this chapter, I decided to include it into this thesis.

We end with a few concluding remarks in chapter 6.

Publication list

This thesis is based on the following articles, as indicated in the beginning of the chapters:

[SG19a] Philip K. Schwartz and Domenico Giulini. 'Post-Newtonian corrections to Schrödinger equations in gravitational fields'. Class. Quantum Grav. **36** (2019), 095016. DOI: `10.1088/1361-6382/ab0fbd`. Corrigendum published in Class. Quantum Grav. **36** (2019), 249502.

[SG19b] Philip K. Schwartz and Domenico Giulini. 'Post-Newtonian Hamiltonian description of an atom in a weak gravitational field'. Phys. Rev. A **100** (2019), 052116. DOI: `10.1103/PhysRevA.100.052116`

[SG20] Philip K. Schwartz and Domenico Giulini. *Classical perspectives on the Newton–Wigner position observable*. 2020. arXiv: `2004.09723 [math-ph]`

2. Geometric structures for post-Newtonian expansions

In an arbitrary general-relativistic[1] spacetime, the concept of a 'post-Newtonian expansion' does not exist *per se*: to make sense of it, we need to introduce certain background structures that give meaning to notions like 'weak gravitational fields' and 'slow velocities' of objects in the spacetime. This chapter will be devoted to the introduction of such structures and the description of our post-Newtonian expansion framework, which will be used in the subsequent chapters. We also use this chapter to introduce some further notations and conventions.

This chapter is partly based on the sections introducing the corresponding concepts in [SG19b], and also incorporates material from [SG19a].

2.1. General conventions

We use the 'mostly plus' $(-+++)$ signature convention for the spacetime metric and stick, as indicated, to four dimensions. However, in many places our work has a straightforward generalisation to higher dimensions. The velocity of light will be denoted by c, and *not* set equal to 1.

When talking about Minkowski spacetime, we will view it as an affine space or, even more often, as an abstract differentiable manifold endowed with a Lorentzian metric, and not identify it with a vector space, unless otherwise stated.

2.2. Background structures

As soon as gravity is geometrised in a metric sense, it does not make sense to speak of the 'absence' of gravitational fields[2], and therefore also not of their 'weakness' – this can only be spoken of with respect to some background metric to compare the physical metric to. This background metric then defines the concept of 'absence' of gravity.

[1] Or described by any other metric theory of gravity.

[2] This is not necessarily true in all geometric theories of gravitation. For example, in teleparallel gravity theories, inertial and gravitational effects can be naturally separated [Per14].

In order to perform a Newtonian limit and to analyse the behaviour of physical systems and theories near this Newtonian limit – that is, to perform a post-Newtonian expansion – we also need some means of decomposing spacetime into 'space' and 'time'. The general idea is that such a decomposition of the background spacetime can be accomplished by considering a 'time evolution' vector field, i.e. a vector field that is, with respect to the background metric, timelike, of constant Lorentzian length, and hypersurface orthogonal. We can then consider the integral curves of this vector field as 'time', and the leaves of the orthogonal distribution as 'space'.

Since we want the geodesic structure of the background spacetime, and its decomposition into space and time, to be compatible with Newtonian concepts, we will take as the background spacetime four-dimensional Minkowski spacetime (M, η) and as 'time evolution' vector field a timelike geodesic vector field u on (M, η). Here η denotes the Minkowski metric. For reasons of physical dimensionality, we assume u to have Minkowski square $\eta(u, u) = -c^2$. We also fix, once and for all, an orientation and a time orientation on Minkowski spacetime, and assume u to be future-directed. Sometimes, we will interpret u as the four-velocity vector field of a family of inertial observers in background Minkowski spacetime.

That the gravitational field be weak now means that the physical spacetime metric on M, which we denote by g, deviate only little from the background Minkowski metric η. The notion of 'deviating only little' will be made more precise in the following section. As described above, we now use η and the preferred timelike vector field u to decompose spacetime into time (integral curves of u) and space (hyperplanes η-orthogonal to u). We endow 'space' with a flat Riemannian metric δ, the restriction of η to the hyperplanes, such that it just becomes ordinary flat Euclidean space. Interpreted as a tensor on four-dimensional spacetime (which annihilates the time direction u and may therefore also be viewed as a purely 'spatial' object), δ can be expressed in geometric, coordinate-free language as

$$\delta := \eta + c^{-2}\, u^\flat \otimes u^\flat \,, \tag{2.2.1}$$

where $u^\flat := \eta(u, \cdot)$ denotes the one-form corresponding to u via the metric. The time evolution vector field u also allows us to define a notion of small / 'slow' velocities – namely spatial velocities, as seen from an observer moving along u, being small compared to c.

We are free to use the 'flat' structure of spacetime and space introduced by the background structures to perform all our computations. However, once results are established, we have to keep in mind that physical distances and times are measured with the physical metric g, not the auxiliary metric η. We will see that in some cases it is precisely such a re-interpretation in terms of the physical metric that lends the results good physical meaning.

For later use, we introduce the 'physical spatial metric' ${}^{(3)}g$, which is the restriction of the physical spacetime metric g to three-dimensional 'space', i.e. to the orthogonal complement of the preferred vector field u. The inverse of this physical spatial metric will be denoted by ${}^{(3)}g^{-1}$.

Let us stress here that all the structures introduced and all the conditions of 'weakness' and 'slowness' mentioned are entirely independent of coordinates that we may choose. That is not to say that there may not be preferred coordinates which are particularly adapted to the given background structure. Indeed, such adapted coordinates obviously exist, namely positively oriented inertial coordinates (x^0, x^1, x^2, x^3) in Minkowski spacetime (M, η), with respect to some arbitrarily chosen origin, such that $x^0 = ct$, $u = \partial/\partial t$, and $\eta = \eta_{\mu\nu}\, \mathrm{d}x^\mu \otimes \mathrm{d}x^\nu$ with $(\eta_{\mu\nu}) = \mathrm{diag}(-1, 1, 1, 1)$. Unless otherwise stated, we will always work in such coordinates adapted to the background structures when dealing with post-Newtonian expansions.

2.3. Further geometric notation and conventions

In our calculations, vectors and tensors will be represented by their components with respect to the chosen coordinate system $(x^\mu) = (ct, x^a)$. We let Greek indices run from 0 to 3 and Latin indices from 1 to 3, and we shall use the Einstein summation convention for like indices at different levels (one up- and one downstairs). Indices are lowered and raised by the physical spacetime metric $g_{\mu\nu}$ and its inverse $g^{\mu\nu}$, respectively. The Minkowski metric takes its usual diagonal form, as stated above. The spatial metric δ induced by the background structures has the usual Euclidean form with components $(\delta_{ab}) = \mathrm{diag}(1, 1, 1)$, and its inverse has components $(\delta^{ab}) = \mathrm{diag}(1, 1, 1)$.

We will often employ a 'three-vector' notation, where the three-tuple of spatial components of some geometric object will be denoted by a boldface letter: for example, $\boldsymbol{v} = (v^1, v^2, v^3)$ is the 'vector' of spatial components of some tangent vector v on M, or $\boldsymbol{A} = (A_1, A_2, A_3)$ the 'vector' of spatial components of some one-form A. When using this notation, a dot between two such 'vectors' will denote the *component-wise* 'Euclidean scalar product', i.e.

$$\boldsymbol{v} \cdot \boldsymbol{w} := \delta_{ab} v^a w^b = \sum_{a=1}^{3} v^a w^a \tag{2.3.1}$$

or

$$\boldsymbol{v} \cdot \boldsymbol{A} := v^a A_a = \sum_{a=1}^{3} v^a A_a \, . \tag{2.3.2}$$

Note that the latter does not depend on δ in the formula, but nevertheless relies on the $3+1$ split induced by the background structures. Similarly, a cross multiplication symbol will denote the *component-wise* vector product, i.e.

$$(\boldsymbol{v} \times \boldsymbol{w})^a := \delta^{an}\, {}^{(3)}\varepsilon_{nbc} v^b w^c \tag{2.3.3}$$

where ${}^{(3)}\varepsilon_{abc}$ is the usual three-dimensional totally antisymmetric symbol. Geometrically, ${}^{(3)}\varepsilon_{abc}$ can be understood as the components of the spatial volume form induced by the Euclidean metric δ. We will lower and raise the indices of ${}^{(3)}\varepsilon$ by δ_{ab} and δ^{ab} respectively, i.e. ${}^{(3)}\varepsilon^a{}_{bc} := \delta^{an}\, {}^{(3)}\varepsilon_{nbc}$ etc., such that we can write $(\boldsymbol{v} \times \boldsymbol{w})^a = {}^{(3)}\varepsilon^a{}_{bc} v^b w^c$.

A boldface nabla symbol $\boldsymbol{\nabla}$ denotes the three-tuple of *partial* derivatives

$$\boldsymbol{\nabla} = (\partial_1, \partial_2, \partial_3), \tag{2.3.4}$$

which can be geometrically understood as the component representation of the spatial covariant derivatives with respect to the flat Euclidean metric. It will be used to express component-wise vector calculus operations in the usual short-hand notation, for example writing

$$(\boldsymbol{\nabla} \times \boldsymbol{A})^a = {}^{(3)}\varepsilon^{abc} \partial_b A_c \tag{2.3.5}$$

for the component-wise curl of $\boldsymbol{A}$.

In view of the structures introduced, we stress again that all the operations reported here and used in the sequel make good geometric sense. They do depend on the geometric structures that we made explicit above, i.e. on the background metric η and the time evolution vector field u, but they do not depend on the coordinates or frames that one uses in order to express the geometric objects (including the background structures) in terms of their real-valued components.

2.4. Formal expansions in c^{-1}

In order to perform a post-Newtonian expansion, we need some means to keep track of 'how far away' from the Newtonian limit some term in a calculation is. A convenient way for doing so is to expand all relevant quantities as formal power series in c^{-1}, i.e. in the inverse of the velocity of light. A term of order c^0 then corresponds to the Newtonian limit of the considered quantity, and the higher-order terms give higher and higher orders of post-Newtonian 'corrections'. Even though it might at first sight seem somewhat peculiar to perform an expansion in a dimensionful quantity, there is nothing to worry about when using this as a method to just formally keep track of post-Newtonian effects, since no questions of convergence ever arise. Note that the Newtonian limit of a quantity corresponds to formally taking the limit $c \to \infty$ in the power series. A quantity X being of order (at least) k in the formal c^{-1}-expansion will be denoted by

$$X = \mathrm{O}(c^{-k}). \tag{2.4.1}$$

Let us again stress that this does not entail any analytic statement at all; it is just a notation for orders in formal power series. To put it differently, we view a post-Newtonian theory as a (formal) deformation of its 'Newtonian limit', implementing the deformation of Galilei to Poincaré symmetry well-known at the level of Lie algebras [İW53].

Sometimes, we will need to consider quantities incorporating terms of *negative* order in c^{-1} (i.e. of positive order in c). However, we will always encounter but finitely many[3] negative-order terms, meaning that we are considering formal Laurent series in the expansion parameter c^{-1}. Note that no Newtonian limit exists for a quantity with non-vanishing such negative-order terms.

In the Newtonian limit, coordinate time[4] t shall be identified with Newtonian absolute time. Therefore, we have to treat t as being of order c^0 in our formal expansion, instead of the timelike coordinate $x^0 = ct$ with dimension of length: were we to take x^0 to be of order c^0, then $t = c^{-1}x^0$ would vanish in the Newtonian limit. However, to the spatial coordinates (x^a) we assign order c^0. This necessity of treating the time direction differently is, of course, well-known: it arises whenever one wants to obtain well-defined Newtonian limits of (locally) Poincaré-relativistic theories, for example in the context of Newton–Cartan theory [Ehl81; Ehl19].

Considering the background Minkowski metric

$$\eta = \eta_{\mu\nu}\,\mathrm{d}x^\mu \otimes \mathrm{d}x^\nu = -c^2\mathrm{d}t^2 + \mathrm{d}\boldsymbol{x}^2, \tag{2.4.2}$$

we see that, due to our treating differently the time coordinate, it consists of terms of different order in c^{-1}: a temporal part of order c^2, and a spatial part of order c^0. This analogously goes for the inverse Minkowski metric

$$\eta^{-1} = -c^{-2}\frac{\partial}{\partial t} \otimes \frac{\partial}{\partial t} + \delta^{ab}\frac{\partial}{\partial x^a} \otimes \frac{\partial}{\partial x^b}\ . \tag{2.4.3}$$

We now turn to the description of the formal c^{-1}-expansion of the *physical* spacetime metric g, which is to make precise the notion of g deviating only little from the Minkowski background η. For the computations in chapter 3, it turns out that it is notationally easiest to label the coefficients in the expansion of the components of the

[3] In fact, only up to order c^4.

[4] Even though we call it 'coordinate time' here, t can of course be characterised in a coordinate-free way as the evolution parameter of integral curves of the background time evolution vector field u.

inverse metric, instead of the metric itself: we expand the components of the inverse metric as formal power series

$$g^{\mu\nu} = \eta^{\mu\nu} + \sum_{k=1}^{\infty} c^{-k} g^{\mu\nu}_{(k)} \,, \tag{2.4.4}$$

the lowest-order term being given by the components of the inverse Minkowski metric. Note that the coefficients in (2.4.4) refer to the coordinates $(x^\mu) = (ct, x^a)$. Thus, when considering the inverse metric proper (and not its components), we obtain

$$\begin{aligned} g^{-1} &= g^{\mu\nu} \frac{\partial}{\partial x^\mu} \otimes \frac{\partial}{\partial x^\nu} \\ &= \eta^{-1} + \sum_{k=1}^{\infty} c^{-k} \left[c^{-2} g^{00}_{(k)} \frac{\partial}{\partial t} \otimes \frac{\partial}{\partial t} + c^{-1} g^{0a}_{(k)} \frac{\partial}{\partial t} \vee \frac{\partial}{\partial x^a} + g^{ab}_{(k)} \frac{\partial}{\partial x^a} \otimes \frac{\partial}{\partial x^b} \right] : \end{aligned} \tag{2.4.5}$$

Coefficients carrying the same notational order label '(k)' appear in different orders of the formal expansion of the proper geometric object g^{-1}. For the sake of notational convenience, we also define

$$g^{-1}_{(k)} := g^{\mu\nu}_{(k)} \frac{\partial}{\partial x^\mu} \otimes \frac{\partial}{\partial x^\nu} \,, \tag{2.4.6}$$

to which the same observation applies.

In chapter 4, we will discuss electromagnetic quantities. In that context, we will treat the electromagnetic four-potential form A and the four-current density j as being of formal expansion order c^0 when considered as tensor (density) fields. Their components with respect to our adapted coordinate system are then of the orders

$$A_0 = \mathrm{O}(c^{-1}),\ A_a = \mathrm{O}(c^0),\ j^0 = \mathrm{O}(c^1),\ j^a = \mathrm{O}(c^0), \tag{2.4.7}$$

factors of c arising in them from $x^0 = ct$ involving a factor of c. This implies that the electric potential $\phi_{\mathrm{el.}} = -cA_0$ and the charge density $\rho = \frac{1}{c} j^0$ are again quantities[5] of order c^0. In particular, for the (non-vanishing) components of the electromagnetic field tensor $F = \mathrm{d}A$, we have $F_{a0} = \mathrm{O}(c^{-1})$ and $F_{ab} = \mathrm{O}(c^0)$.

To ensure consistency in the treatment of expansion orders when dealing with electromagnetism, we will write equations in terms of the vacuum permittivity ε_0 only, to which we assign the formal order $\varepsilon_0 = \mathrm{O}(c^0)$, and avoid usage of the vacuum permeability $\mu_0 = 1/(\varepsilon_0 c^2)$ altogether.

[5] In fact, they are – apart from the conventional minus sign in $\phi_{\mathrm{el.}}$ – simply the t components of the fields with respect to the coordinates (t, x^a).

2.5. The Eddington–Robertson parametrised post-Newtonian metric

One of the easiest and most important physically relevant post-Newtonian metrics is the Eddington–Robertson parametrised post-Newtonian metric, whose components are given by

$$(g_{\mu\nu}) = \begin{pmatrix} -1 - 2\frac{\phi}{c^2} - 2\beta\frac{\phi^2}{c^4} + \mathrm{O}(c^{-6}) & \mathrm{O}(c^{-5}) \\ \mathrm{O}(c^{-5}) & (1 - 2\gamma\frac{\phi}{c^2})\mathbb{1} + \mathrm{O}(c^{-4}) \end{pmatrix}, \tag{2.5.1}$$

where ϕ is a scalar function on spacetime that may be seen as the analogue of the Newtonian gravitational potential in this approximation scheme.

The metric also contains two dimensionless parameters β and γ, the so-called 'Eddington–Robertson parameters'. These account for possible deviations from general relativity, which corresponds to the values $\beta = \gamma = 1$. In that case, the metric (2.5.1) solves the Einstein field equations of general relativity approximately in a c^{-1}-expansion for a static source, with ϕ being the Newtonian gravitational potential of the source. The metrics for different values of these parameters are then considered to correspond to so-called 'test theories' against which the predictions of general relativity can be tested.

In fact, the Eddington–Robertson PPN metric (PPN = 'parametrised post-Newtonian') is just the simplest of a much bigger family of PPN metrics, encompassing a large range of lowest-order post-Newtonian effects of metric theories of gravity and thus offering a large set of theories to test general relativity against. For an extensive discussion of the parametrised post-Newtonian formalism and its applications in tests of gravitational theory, we recommend the monograph [Wil93].

The explicit inclusion of β and γ allows us to track the consequences of post-Newtonian corrections in the spatial and the temporal part of the metric separately. It also opens the possibility to apply our results to potential future quantum tests of general relativity itself, which are, however, outside the scope of this thesis.

Note that even though in its true post-Newtonian origin the function ϕ appearing in the Eddington–Robertson PPN metric is time-independent, we will allow for it to depend on time for the sake of higher generality.

The components of the inverse metric to g are easily obtained as

$$(g^{\mu\nu}) = \begin{pmatrix} -1 + 2\frac{\phi}{c^2} + (2\beta - 4)\frac{\phi^2}{c^4} + \mathrm{O}(c^{-6}) & \mathrm{O}(c^{-5}) \\ \mathrm{O}(c^{-5}) & (1 + 2\gamma\frac{\phi}{c^2})\mathbb{1} + \mathrm{O}(c^{-4}) \end{pmatrix}. \tag{2.5.2}$$

3. Post-Newtonian corrections to Schrödinger equations in gravitational fields

In this chapter, we deal with systematic methods to couple single, free quantum particles to post-Newtonian gravitational fields. More specifically, we extend a WKB-like post-Newtonian expansion of the minimally coupled Klein–Gordon equation after Kiefer and Singh [KS91], Lämmerzahl [Läm95], and Giulini and Großardt [GG12] to arbitrary order in c^{-1}, leading to Schrödinger equations describing a free quantum particle in a general gravitational field in post-Newtonian expansion. We will compare the results of this approach to canonical quantisation of a free particle in curved spacetime, following Wajima *et al.* [WKF97].

Furthermore, using a more 'formal', operator-algebraic approach, expansions of the Klein–Gordon equation and the canonical quantisation method are shown to lead to the same results for terms in the Hamiltonian up to linear order in particle momentum, when the particle is described with respect to a stationary time evolution vector field in a stationary spacetime. For this, no expansion in the inverse of the velocity of light has to be employed. This result means in particular that the lowest-order coupling to gravitomagnetism is described in the same way by both methods.

The material in this chapter has been published in [SG19a].

3.1. Introduction

In the existing literature, one finds two different main approaches to the problem of post-Newtonian 'correction terms' for the Schrödinger equation describing a free quantum particle in a curved spacetime. The first, described, e.g., by Wajima *et al.* [WKF97], starts from a classical description of the particle and applies canonical quantisation rules adapted to the situation (in a somewhat *ad hoc* fashion) to derive a quantum-mechanical Hamiltonian. By an expansion in powers of c^{-1} (at the stage of the classical

Hamiltonian), one finds the desired correction terms. Other intimately related methods use path integral quantisation on the classical system, as, e.g., the semi-classical calculation by Dimopoulos *et al.* [Dim+08]. As discussed in the introduction, such a semi-classical path integral perspective is the most widely used method for the description of gravitational coupling in quantum optics.

The second, fundamentally different approach takes a field-theoretic perspective and derives the Schrödinger equation as an equation for the positive frequency solutions of the minimally coupled classical Klein–Gordon equation. This is accomplished by Kiefer and Singh [KS91], Lämmerzahl [Läm95], and Giulini and Großardt [GG12] by making a WKB-like ansatz for the Klein–Gordon field, thereby formally expanding the Klein–Gordon equation in powers of c^{-1}, in the end viewing the Klein–Gordon theory as a formal deformation of the Schrödinger theory, as explained before in section 2.4. This second method seems to be more firmly rooted in first principles than the canonical quantisation method, since it can at least heuristically be motivated from quantum field theory in curved spacetimes (see section 3.3). In a similar vein, one can apply such expansion methods to the Dirac equation, leading to a proper treatment of fermionic particles.

Although the two methods for obtaining post-Newtonian Schrödinger equations described above are very different in spirit, they lead to comparable results in lowest orders. To make possible a general comparison beyond the explicit examples considered in the existing literature[1], we will apply the methods to as general a metric as possible. In section 3.2, we will give a brief overview over the canonical quantisation method (and extend it to the case of time-dependent metrics). After a heuristic quantum-field-theoretic motivation for considering the classical Klein–Gordon equation in the description of single quantum particles in section 3.3, section 3.4 will develop the WKB-like formal expansion of the Klein–Gordon equation to arbitrary order in c^{-1} in a general metric given as a formal power series in c^{-1}, significantly extending existing explicit examples to the general case. This leads to some simple comparisons of the resulting Hamiltonian with the one coming from canonical quantisation.

In section 3.5, we consider a formal expansion of the Klein–Gordon equation in powers of momentum operators leading to a Schrödinger form of the equation. This yields a general statement about agreement between the canonical and the Klein–Gordon methods for terms in the Hamiltonian up to linear order in momentum in the case of a stationary spacetime, without any necessity of an expansion in powers of c^{-1}.

A similar general WKB-like post-Newtonian formal expansion of the Klein–Gordon equation to obtain a Schrödinger equation was already considered by Tagirov in [Tag90]

[1] Wajima *et al.* [WKF97] considered a first-order post-Newtonian metric for a point-like rotating source, Lämmerzahl [Läm95] used the first-order Eddington–Robertson PPN metric.

and a series of follow-up papers [Tag92; Tag96], as summarised in [Tag99]; but unlike our approach, these works did not expand the metric, thus not allowing to directly apply the results to metrics given as a power series in c^{-1}. Tagirov also compared his WKB-like approach to methods of canonical quantisation [Tag03], but did this only for the case of static metrics.

Since we are concerned mostly with conceptual questions, we will generally not be mathematically very rigorous in this chapter, and in particular not mention domains of definition of operators.

3.2. Canonical quantisation of a free particle

In the following, we will describe the canonical quantisation approach that was used by Wajima *et al.* [WKF97] to derive a Hamiltonian for a quantum particle in the post-Newtonian gravitational field of a point-like rotating source. We will allow metrics as general as possible, and focus on the conceptual issues of the procedure when adapted to our geometric framework from chapter 2. We will also extend the procedure such that we are able to define a quantum theory in the case of a time-dependent metric.

The classical action for a 'relativistic' point particle of mass m in curved spacetime with metric g is

$$S = -mc \int \mathrm{d}\lambda \, \sqrt{-g(x'(\lambda), x'(\lambda))} = -mc \int \mathrm{d}\lambda \, \sqrt{-g_{\mu\nu} x'^{\mu} x'^{\nu}} \,, \tag{3.2.1}$$

where $x(\lambda)$ is the arbitrarily parametrised worldline of the particle. Parametrising the worldline by coordinate time $t = x^0/c$, i.e. 'background time' measured along the background time evolution vector field u as introduced in section 2.2, the classical Hamiltonian for t-evolution can be computed to be

$$H = \frac{1}{\sqrt{-g^{00}}} c \left[m^2 c^2 + \left(g^{ab} - \frac{1}{g^{00}} g^{0a} g^{0b} \right) p_a p_b \right]^{1/2} + \frac{c}{g^{00}} g^{0a} p_a \tag{3.2.2}$$

when expressed in terms of the components of the (inverse) spacetime metric, where p_a are the momenta conjugate to x^a. Full details of this calculation can be found in appendix A.

Note that this Hamiltonian formalism makes use of the decomposition of spacetime into space and time as induced by the background structures. In the following, we will denote the spacelike leaf of 'space' at background time t, as given by the background structures, by $\Sigma_t \subset M$. The 'spaces' corresponding to different values of t may naturally be identified along the flow of the background time evolution vector field, which in our adapted coordinates is just given by identifying points with the same spatial coordinates, i.e. $(ct_1, x^a) \mapsto (ct_2, x^a)$. The quotient space, which may be viewed as 'abstract' Euclidean three-space proper, will be denoted by Σ, and there is a natural embedding $\Sigma \xrightarrow{\cong} \Sigma_t \subset M$ for each t. Of course, all of this depends on the background structures, and thus will the quantum theory we are about to construct[2].

Now, we want to 'canonically quantise' the classical Hamiltonian (3.2.2). To this end, we expand the square root in (3.2.2) to the desired order in c^{-1} (or in momenta, see section 3.5), and afterwards replace the classical momentum and position variables by corresponding operators, satisfying the canonical commutation relations. Of course, for doing so we have to choose an operator ordering scheme for symmetrising products of momenta and (functions of) position. We thus obtain a quantised Hamiltonian $\hat{H}$, acting on the Hilbert space on which the position and momentum operators are defined, and can postulate a Schrödinger equation in the usual form

$$i\hbar\partial_t\psi = \hat{H}\psi. \tag{3.2.3}$$

Let us stress once more that this Hamiltonian will depend not only on the background structures η, u which define the post-Newtonian approximation, but also on the choice of operator ordering scheme, which we leave open in order to keep the discussion as general as possible.

Note that, according to the Stone–von Neumann theorem, the Hilbert space on which the position and momentum operators act and the form they take are essentially uniquely determined (up to unitary equivalence) by demanding the canonical commutation relations[3]. Thus, the quantum theory is completely specified by the choice of ordering scheme, without any further choice concerning a possible explicit form of the Hilbert space. Nevertheless, we will now discuss explicit realisations of the Hilbert space and the position and momentum operators, in order to gain a more direct geometric interpretation thereof. This will also become important when comparing canonical quantisation to formal expansions of the Klein–Gordon equation in the following sections.

[2] In fact, the constructions of this section can also be applied in a slightly different setting. We could assume the spacetime to be globally hyperbolic and perform a $3+1$ decomposition [Giu14]: we foliate spacetime M into three-dimensional spacelike Cauchy surfaces Σ_t which are images of an 'abstract' Cauchy surface Σ under a family of embeddings $\mathcal{E}_t \colon \Sigma \to M$, parametrised by a 'foliation parameter' $t \in \mathbb{R}$, and introduce spacetime coordinates such that x^a are coordinates on Σ and $x^0 = ct$. In this setting, the embeddings $\mathcal{E}_t$ defining the $3+1$ decomposition would constitute the 'background structure' on which the quantum theory will depend.

[3] Of course, as is well-known, the uniqueness statement is, due to the unboundedness of the operators, only strictly true when considering the 'exponentiated' version of the canonical commutation relations, i.e. the Weyl relations. This essentially amounts to a regularity condition, which we shall also implicitly assume on physical grounds.

Since the position variables in the classical Hamiltonian (3.2.2) are the spatial coordinates x^a on three-dimensional 'space', we want the quantum position operators to directly correspond to these. That is, we want to define the Hilbert space as some space of square-integrable 'wavefunctions' of the x^a, such that we can take as position operators simply the operators of multiplication with the coordinates, thus obtaining a direct interpretation of the 'wavefunctions' in the Hilbert space as 'position probability amplitude distributions'. The question of explicit realisation of the Hilbert space thus becomes a question of choice of a scalar product on (some subspace of) the space of functions of the x^a.

To be more precise, we do not just need a single Hilbert space: to any time t we want to associate a wavefunction $\psi(t)$ giving rise to a position probability distribution *on the spatial leaf* Σ_t *corresponding to* t, so we need to consider an individual Hilbert space for each spatial leaf. But since we want to relate these wavefunctions by a Schrödinger equation, we have to somehow identify the Hilbert spaces corresponding to different times.

A natural, geometric choice of scalar product on the space of functions on Σ_t is the L^2-scalar product with respect to the induced metric measure (compare [WKF97]), i.e.

$$\langle \psi, \varphi \rangle_{\Sigma_t} := \int \mathrm{d}^3\boldsymbol{x}\, \overline{\psi}\varphi \sqrt{{}^{(3)}g|_{\Sigma_t}}\,, \tag{3.2.4}$$

where here and in the following, we use the short-hand notation ${}^{(3)}g = \det(g_{ab})$ for the determinant of the matrix of coordinate components of the spatial metric, when no confusion with the spatial metric ${}^{(3)}g$ proper can arise. Consider first the case that the spatial metric components g_{ab} be independent of t, i.e. that the induced geometry be 'the same' for all spatial leaves (implicitly identifying each Σ_t with 'abstract space' Σ via the natural embedding $\Sigma \overset{\cong}{\to} \Sigma_t$). Then the scalar product (3.2.4) is independent of t, such that the Hilbert spaces corresponding to the different spatial slices are canonically identified by simply identifying the wavefunctions (again identifying $\Sigma_t \cong \Sigma$). We can then define the momentum operator as

$$\hat{p}_a := -\mathrm{i}\hbar\, {}^{(3)}g^{-1/4}\, \partial_a({}^{(3)}g^{1/4}\cdot), \tag{3.2.5}$$

which is symmetric with respect to the scalar product and fulfils the canonical commutation relation $[x^a, \hat{p}_b] = \mathrm{i}\hbar\delta^a_b$, and carry out canonical quantisation as described above.

If we allow for the g_{ab} to depend on t, the scalar product (3.2.4) depends on t and thus the canonical map $\mathrm{L}^2(\Sigma, \langle\cdot,\cdot\rangle_{\Sigma_t}) \ni \psi \mapsto \psi \in \mathrm{L}^2(\Sigma, \langle\cdot,\cdot\rangle_{\Sigma_s})$ no longer is an isomorphism of Hilbert spaces. I.e. the natural identification from above does not work, spoiling the program of canonical quantisation with this concrete realisation / geometric interpretation of the Hilbert spaces. A natural solution to this problem is to instead consider the time-independent 'flat' L^2-scalar product

$$\langle \psi_f, \varphi_f \rangle_f := \int d^3\boldsymbol{x}\, \overline{\psi_f}\, \varphi_f \tag{3.2.6}$$

together with the 'flat' momentum operator $\bar{p}_a := -i\hbar\partial_a$. Using these, we obtain a 'geometric realisation' of our canonical quantisation Hilbert space also in the case of time-dependent g_{ab}. At first sight, this scalar product could seem less 'geometric' than (3.2.4), but it can be seen to have as much invariant meaning as the latter by realising that, geometrically speaking, the 'flat' wavefunctions ψ_f, φ_f be scalar *densities* (of weight 1/2) on Σ instead of scalar functions. Since this choice of 'flat' scalar product can be applied to more general situations, and it eases the comparison to usual Galilei-invariant Schrödinger theory and to the Klein–Gordon expansion methods to be discussed in the following, we will adopt it from now on, i.e. 'canonically quantise' the expanded classical Hamiltonian by replacing the classical momentum by the flat momentum operator (applying our chosen ordering scheme).

As explained above, the two choices of explicit realisation of the Hilbert space that we described for the case of time-independent g_{ab} have to be unitarily equivalent by the Stone–von Neumann theorem. The unitary operator implementing this equivalence can be directly read off from the definitions of the two scalar products, and is given by $\psi \mapsto \psi_f = {}^{(3)}g^{1/4}\,\psi$.

3.3. Formal expansions of the Klein–Gordon equation: heuristic motivation from quantum field theory in stationary spacetimes

In the following, we will consider formal expansions of the classical, minimally coupled Klein–Gordon equation for a particle of mass $m > 0$,

$$\left(\Box - \frac{m^2c^2}{\hbar^2}\right)\Psi_{KG} = 0, \tag{3.3.1}$$

leading to a Schrödinger equation with post-Newtonian corrections. In section 3.4, we shall deal with a WKB-inspired formal expansion in c^{-1}, while in section 3.5, we will draw a comparison to canonical quantisation based on an expansion in spatial momentum. To lay a conceptual foundation for these investigations, we will in this section give a heuristic motivation for consideration of the classical Klein–Gordon equation from quantum field theory in curved spacetimes.

Instead of (3.3.1) one could also consider the more general case of a possibly *non*-minimally coupled Klein–Gordon equation, i.e. including some curvature term. This is customary in modern literature on quantum field theory in curved spacetime, where an additional term $-\xi R \Psi_{\mathrm{KG}}$ is included in the equation, R being the scalar curvature of the spacetime [BF09, eq. (5.57)]. In particular, for the choice of $\xi = \frac{1}{6}$ ('conformal coupling'), the equation becomes conformally invariant in the massless case $m = 0$, and also in the massive case there are some arguments favouring the conformally coupled Klein–Gordon equation, in particular in de Sitter spacetime [Tag73]. Nevertheless, we will for the sake of simplicity stick with the minimally coupled equation in this thesis, leaving non-minimal coupling for possible later investigations.

Now, we turn to the advertised motivation of consideration of the classical Klein–Gordon equation on a heuristic level. Namely, the quantum field theory construction for the free Klein–Gordon field on a globally hyperbolic stationary spacetime proceeds as follows (see, e.g., [Wal94, section 4.3]).

We consider the Klein–Gordon equation (3.3.1) on a general globally hyperbolic stationary spacetime, and the Klein–Gordon inner product, which for two solutions $\Psi_{\mathrm{KG}}, \Phi_{\mathrm{KG}}$ of (3.3.1) is given by

$$\begin{aligned} \langle \Psi_{\mathrm{KG}}, \Phi_{\mathrm{KG}} \rangle_{\mathrm{KG}} &= \mathrm{i}\hbar c \int_\Sigma \mathrm{d}^3\boldsymbol{x}\, \sqrt{{}^{(3)}g}\, n^\nu \left[\overline{\Psi_{\mathrm{KG}}} (\nabla_\nu \Phi_{\mathrm{KG}}) - (\nabla_\nu \overline{\Psi_{\mathrm{KG}}}) \Phi_{\mathrm{KG}} \right] \\ &= \mathrm{i}\hbar c \int_\Sigma \mathrm{d}^3\boldsymbol{x}\, \sqrt{{}^{(3)}g}\, n^\nu \left[\overline{\Psi_{\mathrm{KG}}} (\partial_\nu \Phi_{\mathrm{KG}}) - (\partial_\nu \overline{\Psi_{\mathrm{KG}}}) \Phi_{\mathrm{KG}} \right], \end{aligned} \tag{3.3.2}$$

where Σ is a spacelike Cauchy surface, ${}^{(3)}g$ is the determinant of the induced metric on Σ, and n is the future-directed unit normal vector field of Σ. In the second line, which is valid in a coordinate basis, we used that the covariant derivative of a scalar function is just the ordinary exterior derivative, i.e. given by a partial derivative in the case of a coordinate basis. Using the Klein–Gordon equation and Gauß' theorem, (3.3.2) can be shown to be independent of the choice of Σ under the assumption that the fields satisfy suitable boundary conditions.

The Hilbert space of the quantum field theory is now the bosonic Fock space over the 'one-particle' Hilbert space constructed, loosely speaking, as the completion of the space of classical solutions of the Klein–Gordon equation with 'positive frequency' (with respect to the stationarity Killing field) with the Klein–Gordon inner product.

To be more precise, the construction of the 'one-particle' Hilbert space is a little more involved, since it is not *a priori* clear what is meant by 'positive frequency solutions': at first, the space of classical solutions of the Klein–Gordon equation is completed in a certain inner product to obtain an 'intermediate' Hilbert space on which the generator of time translations (with respect to the stationarity Killing field) can be shown to be a self-adjoint operator; the positive spectral subspace of this operator is then completed in the Klein–Gordon inner product to give the Hilbert space of one-particle states. For details on the construction, see [Wal94, section 4.3] and the references cited therein.

So the one-particle sector of the free Klein–Gordon quantum field theory in globally hyperbolic stationary spacetime is described by an appropriate notion of positive frequency solutions of the classical Klein–Gordon equation, using the Klein–Gordon inner product. Note that in this representation, in which the Klein–Gordon inner product takes its usual form, the 'naive position operator' (multiplying with coordinate position) is the well-known Newton–Wigner position when we are considering Minkowski spacetime.

At this point, the quantum-field-theoretic motivation of our Klein–Gordon expansion methods becomes merely heuristic: since in the following we will not solve the Klein–Gordon equation exactly, but consider formal expansions of it (either in powers of c^{-1} or in powers of spatial momentum), it will not be possible to exactly determine the space of positive frequency solutions according to the procedure described above; instead, we will merely choose an oscillating phase factor such as to guarantee the solution to have positive instead of negative frequency in lowest order in the expansion (see (3.4.20)). If analysed more rigorously, it could turn out that for an asymptotic solution to be of positive frequency in some stricter sense, additional restrictions on the solution have to be made, possibly altering the function space under consideration. I.e. in principle, this could lead to the Hamiltonian we will obtain being altered when considering a rigorous analytic post-Newtonian expansion of quantum field theory in curved spacetime, instead of just a formal power series expansion.

In the non-stationary case, there is no canonical notion of particles and thus, strictly speaking, the whole question about the behaviour of single quantum particles does not make sense. Nevertheless, for an observer moving on an orbit which is approximately Killing, the classical Klein–Gordon theory can, on a heuristic level, still be expected to lead to approximately correct predictions regarding this observer's observations.

Even if this motivation is just a heuristic, the WKB-like approach of expanding the Klein–Gordon equation in powers of c^{-1} will allow us to view the classical Klein–Gordon theory as a formal deformation of the 'non-relativistic' Schrödinger theory, and makes the sense in which that happens formally precise, the same happening for the momentum expansion.

3.4. WKB-like expansion of the Klein–Gordon equation

Now, we will consider WKB-like formal expansions in c^{-1} of the Klein–Gordon equation (3.3.1), as first introduced by Kiefer and Singh in [KS91] for Minkowski spacetime, and later considered by Lämmerzahl in [Läm95] for the simple Eddington–Robertson

PPN metric, and by Giulini and Großardt in [GG12] for general spherically symmetric metrics.

After developing the expansion of the Klein–Gordon equation to arbitrary order in c^{-1}, we will explain the transformation to a 'flat' L^2-scalar product for comparison to canonical quantisation, and finally consider the metric of the Eddington–Robertson PPN test theory as a simple explicit example.

3.4.1. General derivation

We assume the post-Newtonian physical spacetime metric to be given by a formal power series in c^{-1} as in (2.4.4). Let us remind ourselves that we will work in our coordinate system that is adapted to the background structures defining the notion of post-Newtonian expansion.

In coordinates, the d'Alembert operator in a general Lorentzian metric, as acting on scalar functions, is given by

$$\begin{aligned}\Box f &= \nabla^\mu \nabla_\mu f \\ &= \frac{1}{\sqrt{-g}} \partial_\mu \left(\sqrt{-g}\, g^{\mu\nu} \partial_\nu f\right) \\ &= \frac{1}{\sqrt{-g}} (\partial_\mu \sqrt{-g}) g^{\mu\nu} \partial_\nu f + \partial_\mu (g^{\mu\nu}) \partial_\nu f + g^{\mu\nu} \partial_\mu \partial_\nu f, \end{aligned} \tag{3.4.1}$$

where we use the short-hand notation $g = \det(g_{\mu\nu})$ for the determinant of the matrix of coordinate components of the metric, when no confusion with the metric proper can arise. The second and third term in this expression can easily be expanded in c^{-1} by inserting the expansion (2.4.4) of the components of the inverse metric and using $x^0 = ct$: the third term is

$$\begin{aligned} g^{\mu\nu} \partial_\mu \partial_\nu &= -c^{-2} \partial_t^2 + \Delta + \sum_{k=1}^{\infty} c^{-k} g^{00}_{(k)} c^{-2} \partial_t^2 + \sum_{k=1}^{\infty} c^{-k} 2 g^{0a}_{(k)} c^{-1} \partial_t \partial_a + \sum_{k=1}^{\infty} c^{-k} g^{ab}_{(k)} \partial_a \partial_b \\ &= -c^{-2} \partial_t^2 + \Delta + \sum_{k=3}^{\infty} c^{-k} g^{00}_{(k-2)} \partial_t^2 + \sum_{k=2}^{\infty} c^{-k} 2 g^{0a}_{(k-1)} \partial_t \partial_a + \sum_{k=1}^{\infty} c^{-k} g^{ab}_{(k)} \partial_a \partial_b \ , \end{aligned} \tag{3.4.2}$$

where $\Delta = \delta^{ab} \partial_a \partial_b$ denotes the 'flat' Euclidean Laplacian on three-dimensional space, as induced by the background structures. Similarly, the second term evaluates to

$$\begin{aligned} (\partial_\mu g^{\mu\nu}) \partial_\nu = \sum_{k=3}^{\infty} c^{-k} (\partial_t g^{00}_{(k-2)}) \partial_t + \sum_{k=2}^{\infty} c^{-k} (\partial_t g^{0a}_{(k-1)}) \partial_a \\ + \sum_{k=2}^{\infty} c^{-k} (\partial_a g^{0a}_{(k-1)}) \partial_t + \sum_{k=1}^{\infty} c^{-k} (\partial_a g^{ab}_{(k)}) \partial_b \ . \end{aligned} \tag{3.4.3}$$

Since the remaining first term of (3.4.1) involves the expression

$$\frac{1}{\sqrt{-g}}\partial_\mu \sqrt{-g} = \frac{1}{2g}\partial_\mu g = \frac{1}{2} g^{\rho\sigma}\partial_\mu g_{\rho\sigma} = -\frac{1}{2} g_{\rho\sigma}\partial_\mu g^{\rho\sigma}, \tag{3.4.4}$$

we need an expression for the c^{-1}-expansion of the components of the *metric*, not just the inverse metric. Rewriting the expansion of the inverse metric as

$$g^{\mu\nu} = \left[\left(\mathbb{1} + \sum_{k=1}^{\infty} c^{-k} g^{-1}_{(k)}\eta\right)\eta^{-1}\right]^{\mu\nu}, \tag{3.4.5}$$

where we used the objects $g^{-1}_{(k)}$ introduced in (2.4.6), we see that a formal Neumann series can be used to invert the power series. This gives the coefficients of the metric as

$$g_{\mu\nu} = \left\{\eta\left[\mathbb{1} + \sum_{n=1}^{\infty}\left(-\sum_{k=1}^{\infty} c^{-k} g^{-1}_{(k)}\eta\right)^n\right]\right\}_{\mu\nu}. \tag{3.4.6}$$

Iterating the Cauchy product formula, we have

$$\left(-\sum_{k=1}^{\infty} c^{-k} g^{-1}_{(k)}\eta\right)^n = (-1)^n \sum_{k=1}^{\infty} c^{-k} \sum_{\substack{i_1+\cdots+i_n=k\\ 1\le i_1,\ldots,i_n\le k}} g^{-1}_{(i_1)}\eta\cdots g^{-1}_{(i_n)}\eta. \tag{3.4.7}$$

Using this and introducing the notation

$$g^{-1}_{(k,n)} := \sum_{\substack{i_1+\cdots+i_n=k\\ 1\le i_1,\ldots,i_n\le k}} g^{-1}_{(i_1)}\eta g^{-1}_{(i_2)}\eta\cdots g^{-1}_{(i_n)}\,, \tag{3.4.8}$$

we can write the metric as

$$g_{\mu\nu} = \eta_{\mu\nu} + \sum_{k=1}^{\infty} c^{-k}\sum_{n=1}^{\infty}(-1)^n(\eta g^{-1}_{(k,n)}\eta)_{\mu\nu}\,. \tag{3.4.9}$$

Thus, returning to (3.4.4) we obtain, using the Cauchy product formula again,

$$\begin{aligned} g_{\rho\sigma}\partial_\mu g^{\rho\sigma} &= \left(\eta_{\rho\sigma} + \sum_{k=1}^{\infty} c^{-k}\sum_{n=1}^{\infty}(-1)^n(\eta g^{-1}_{(k,n)}\eta)_{\rho\sigma}\right)\sum_{m=1}^{\infty} c^{-m}\partial_\mu g^{\rho\sigma}_{(m)} \\ &= \sum_{k=1}^{\infty} c^{-k}\partial_\mu \operatorname{tr}(\eta g^{-1}_{(k)}) + \sum_{k=2}^{\infty} c^{-k}\sum_{l+m=k}\sum_{n=1}^{\infty}(-1)^n(\eta g^{-1}_{(l,n)}\eta)_{\rho\sigma}\,\partial_\mu g^{\rho\sigma}_{(m)}\,, \end{aligned} \tag{3.4.10}$$

where in the sum $\sum_{l+m=k}$, the summation variables l and m take values ≥ 1, which we notationally suppress here and in the following. Using

$$\begin{aligned}\sum_{l+m=k}(\eta g^{-1}_{(l,n)}\eta)_{\rho\sigma}\,\partial_\mu g^{\rho\sigma}_{(m)} &= \sum_{l+m=k}\;\sum_{i_1+\cdots+i_n=l}(\eta g^{-1}_{(i_1)}\cdots g^{-1}_{(i_n)}\eta)_{\rho\sigma}\,\partial_\mu g^{\rho\sigma}_{(m)}\\ &= \sum_{i_1+\cdots+i_n+m=k}\operatorname{tr}(\eta g^{-1}_{(i_1)}\cdots g^{-1}_{(i_n)}\eta\,\partial_\mu g^{-1}_{(m)})\\ &= \frac{1}{n+1}\,\partial_\mu\sum_{i_1+\cdots+i_n+m=k}\operatorname{tr}(\eta g^{-1}_{(i_1)}\cdots g^{-1}_{(i_n)}\eta g^{-1}_{(m)})\\ &= \frac{1}{n+1}\,\partial_\mu\operatorname{tr}(\eta g^{-1}_{(k,n+1)})\end{aligned} \tag{3.4.11}$$

and the facts that $g^{-1}_{(k,n)} = 0$ for $n > k$ and $g^{-1}_{(k,1)} = g^{-1}_{(k)}$, we can rewrite this as

$$\begin{aligned}g_{\rho\sigma}\partial_\mu g^{\rho\sigma} &= \sum_{k=1}^{\infty}c^{-k}\partial_\mu\operatorname{tr}(\eta g^{-1}_{(k)}) + \sum_{k=2}^{\infty}c^{-k}\sum_{n=2}^{\infty}(-1)^{n-1}\frac{1}{n}\,\partial_\mu\operatorname{tr}(\eta g^{-1}_{(k,n)})\\ &= \sum_{k=1}^{\infty}c^{-k}\partial_\mu\operatorname{tr}(\eta g^{-1}_{(k)}) + \sum_{k=1}^{\infty}c^{-k}\sum_{n=2}^{\infty}(-1)^{n-1}\frac{1}{n}\,\partial_\mu\operatorname{tr}(\eta g^{-1}_{(k,n)})\\ &= \sum_{k=1}^{\infty}c^{-k}\sum_{n=1}^{\infty}(-1)^{n-1}\frac{1}{n}\,\partial_\mu\operatorname{tr}(\eta g^{-1}_{(k,n)}).\end{aligned} \tag{3.4.12}$$

Thus, we finally obtain the expansion

$$\begin{aligned}&\frac{1}{\sqrt{-g}}(\partial_\mu\sqrt{-g})g^{\mu\nu}\partial_\nu f\\ &\quad= -\frac{1}{2}(g_{\rho\sigma}\,\partial_\mu g^{\rho\sigma})g^{\mu\nu}\partial_\nu f\\ &\quad= \frac{1}{2}\sum_{k=1}^{\infty}c^{-k}\sum_{n=1}^{\infty}(-1)^n\frac{1}{n}[\partial_\mu\operatorname{tr}(\eta g^{-1}_{(k,n)})]\left(\eta^{\mu\nu} + \sum_{m=1}^{\infty}c^{-m}g^{\mu\nu}_{(m)}\right)\partial_\nu f\\ &\quad= \frac{1}{2}\sum_{k=1}^{\infty}c^{-k}\sum_{n=1}^{\infty}(-1)^n\frac{1}{n}[\partial_\mu\operatorname{tr}(\eta g^{-1}_{(k,n)})]\,\eta^{\mu\nu}\partial_\nu f\\ &\qquad+ \frac{1}{2}\sum_{k=2}^{\infty}c^{-k}\sum_{l+m=k}\;\sum_{n=1}^{\infty}(-1)^n\frac{1}{n}[\partial_\mu\operatorname{tr}(\eta g^{-1}_{(l,n)})]\,g^{\mu\nu}_{(m)}\partial_\nu f\end{aligned} \tag{3.4.13}$$

for the first term in the d'Alembert operator (3.4.1).

Inserting (3.4.2), (3.4.3), and (3.4.13) into (3.4.1) and sorting the sums by order of c^{-1}, the full expansion of the d'Alembert operator reads

$$\begin{aligned}\Box f = &\frac{1}{2}\sum_{k=4}^{\infty} c^{-k} \sum_{l+m=k-2} \sum_{n=1}^{\infty} (-1)^n \frac{1}{n} g^{00}_{(m)} [\partial_t \operatorname{tr}(\eta g^{-1}_{(l,n)})]\, \partial_t f \\
&+ \frac{1}{2}\sum_{k=3}^{\infty} c^{-k} \sum_{l+m=k-1} \sum_{n=1}^{\infty} (-1)^n \frac{1}{n} g^{0a}_{(m)} \left([\partial_t \operatorname{tr}(\eta g^{-1}_{(l,n)})]\, \partial_a f + [\partial_a \operatorname{tr}(\eta g^{-1}_{(l,n)})]\, \partial_t f \right) \\
&- \frac{1}{2}\sum_{k=3}^{\infty} c^{-k} \sum_{n=1}^{\infty} (-1)^n \frac{1}{n} [\partial_t \operatorname{tr}(\eta g^{-1}_{(k-2,n)})]\, \partial_t f \\
&+ \sum_{k=3}^{\infty} c^{-k} (\partial_t g^{00}_{(k-2)})\, \partial_t f + \sum_{k=3}^{\infty} c^{-k} g^{00}_{(k-2)} \partial_t^2 f \\
&+ \frac{1}{2}\sum_{k=2}^{\infty} c^{-k} \sum_{l+m=k} \sum_{n=1}^{\infty} (-1)^n \frac{1}{n} g^{ab}_{(m)} [\partial_a \operatorname{tr}(\eta g^{-1}_{(l,n)})]\, \partial_b f \\
&+ \sum_{k=2}^{\infty} c^{-k} \left((\partial_t g^{0a}_{(k-1)})\, \partial_a f + (\partial_a g^{0a}_{(k-1)})\, \partial_t f \right) + \sum_{k=2}^{\infty} c^{-k}\, 2 g^{0a}_{(k-1)} \partial_t \partial_a f - c^{-2} \partial_t^2 f \\
&+ \frac{1}{2}\sum_{k=1}^{\infty} c^{-k} \sum_{n=1}^{\infty} (-1)^n \frac{1}{n} [\partial_a \operatorname{tr}(\eta g^{-1}_{(k,n)})] \delta^{ab} \partial_b f \\
&+ \sum_{k=1}^{\infty} c^{-k} (\partial_a g^{ab}_{(k)}) \partial_b f + \sum_{k=1}^{\infty} c^{-k} g^{ab}_{(k)} \partial_a \partial_b f + \Delta f. \end{aligned} \tag{3.4.14}$$

Now, we make the WKB-like ansatz

$$\Psi_{\mathrm{KG}} = \exp\left(\frac{\mathrm{i}c^2}{\hbar} S\right) \psi,\ \psi = \sum_{k=0}^{\infty} c^{-k} a_k \tag{3.4.15}$$

for the Klein–Gordon field (compare [GG12]), where S is a *real* function; i.e. we separate off a phase factor and expand the remainder as a power series in c^{-1}. All the functions S, a_k are assumed to be independent of the expansion parameter c^{-1}. The derivatives of the field are

$$\partial_\mu \Psi_{\mathrm{KG}} = \frac{\mathrm{i}c^2}{\hbar} (\partial_\mu S) \Psi_{\mathrm{KG}} + \exp(\ldots) \partial_\mu \psi \tag{3.4.16}$$

and

$$\begin{aligned}\partial_\mu \partial_\nu \Psi_{\mathrm{KG}} = \exp\left(\frac{\mathrm{i}c^2}{\hbar} S\right) \bigg(&-\frac{c^4}{\hbar^2} (\partial_\mu S)(\partial_\nu S) \psi + \frac{\mathrm{i}c^2}{\hbar} \big[(\partial_\mu \partial_\nu S) \psi \\
&+ (\partial_\mu S) \partial_\nu \psi + (\partial_\nu S) \partial_\mu \psi \big] + \partial_\mu \partial_\nu \psi \bigg). \end{aligned} \tag{3.4.17}$$

Using these and the expansion (3.4.14) of the d'Alembert operator, we can now analyse the Klein–Gordon equation (3.3.1) order by order in c^{-1}. At the lowest occurring order c^4, we get

$$-\exp\left(\frac{\mathrm{i}c^2}{\hbar}S\right)\frac{1}{\hbar^2}\delta^{ab}(\partial_a S)(\partial_b S)a_0 = 0, \tag{3.4.18}$$

which is equivalent[4] to $\partial_a S = 0$. So S is a function of (coordinate) time only. Using this, the Klein–Gordon equation has no term of order c^3.

At c^2, we get

$$\exp\left(\frac{\mathrm{i}c^2}{\hbar}S\right)\left(\frac{1}{\hbar^2}(\partial_t S)^2 - \frac{m^2}{\hbar^2}\right)a_0 = 0, \tag{3.4.19}$$

equivalent to $\partial_t S = \pm m$. Since we are interested in positive-frequency solutions of the Klein–Gordon equation, we choose $\partial_t S = -m$, leading to

$$S = -mt \tag{3.4.20}$$

(an additional constant term would lead to an irrelevant global phase).

The c^1 coefficient leads to the equation

$$-\exp\left(\frac{\mathrm{i}c^2}{\hbar}S\right)g^{00}_{(1)}\frac{m^2}{\hbar^2}a_0 = 0, \tag{3.4.21}$$

equivalent to

$$g^{00}_{(1)} = 0. \tag{3.4.22}$$

Thus the requirement that the Klein–Gordon equation have solutions which are formal power series of the form (3.4.15) imposes restrictions on the components of the metric. In the following, we will freely use the vanishing of $g^{00}_{(1)}$.

[4] For nontrivial solutions, i.e. $a_0 \neq 0$.

Using (3.4.20) and (3.4.22), the positive frequency Klein–Gordon equation for our WKB-like solutions is equivalent to the following equation for ψ:

$$\begin{aligned}
0 = &\sum_{k=5}^{\infty} c^{-k} \frac{1}{2} \sum_{l+m=k-2} \sum_{n=1}^{\infty} (-1)^n \frac{1}{n} g^{00}_{(m)} [\partial_t \operatorname{tr}(\eta g^{-1}_{(l,n)})] \, \partial_t \psi \\
&+ \sum_{k=4}^{\infty} c^{-k} (\partial_t g^{00}_{(k-2)}) \, \partial_t \psi + \sum_{k=4}^{\infty} c^{-k} g^{00}_{(k-2)} \partial_t^2 \psi \\
&- \sum_{k=3}^{\infty} c^{-k} \frac{\mathrm{i}m}{2\hbar} \sum_{l+m=k} \sum_{n=1}^{\infty} (-1)^n \frac{1}{n} g^{00}_{(m)} [\partial_t \operatorname{tr}(\eta g^{-1}_{(l,n)})] \psi \\
&+ \sum_{k=3}^{\infty} c^{-k} \frac{1}{2} \sum_{l+m=k-1} \sum_{n=1}^{\infty} (-1)^n \frac{1}{n} g^{0a}_{(m)} \Big([\partial_t \operatorname{tr}(\eta g^{-1}_{(l,n)})] \, \partial_a \psi + [\partial_a \operatorname{tr}(\eta g^{-1}_{(l,n)})] \, \partial_t \psi \Big) \\
&- \sum_{k=3}^{\infty} c^{-k} \frac{1}{2} \sum_{n=1}^{\infty} (-1)^n \frac{1}{n} [\partial_t \operatorname{tr}(\eta g^{-1}_{(k-2,n)})] \, \partial_t \psi \\
&- \sum_{k=2}^{\infty} c^{-k} \frac{\mathrm{i}m}{\hbar} (\partial_t g^{00}_{(k)}) \psi - \sum_{k=2}^{\infty} c^{-k} \frac{2\mathrm{i}m}{\hbar} g^{00}_{(k)} \partial_t \psi \\
&+ \sum_{k=2}^{\infty} c^{-k} \frac{1}{2} \sum_{l+m=k} \sum_{n=1}^{\infty} (-1)^n \frac{1}{n} g^{ab}_{(m)} [\partial_a \operatorname{tr}(\eta g^{-1}_{(l,n)})] \, \partial_b \psi \\
&+ \sum_{k=2}^{\infty} c^{-k} \Big((\partial_t g^{0a}_{(k-1)}) \, \partial_a \psi + (\partial_a g^{0a}_{(k-1)}) \, \partial_t \psi \Big) + \sum_{k=2}^{\infty} c^{-k} \, 2 g^{0a}_{(k-1)} \partial_t \partial_a \psi - c^{-2} \partial_t^2 \psi \\
&- \sum_{k=1}^{\infty} c^{-k} \frac{\mathrm{i}m}{2\hbar} \sum_{l+m=k+1} \sum_{n=1}^{\infty} (-1)^n \frac{1}{n} g^{0a}_{(m)} [\partial_a \operatorname{tr}(\eta g^{-1}_{(l,n)})] \psi \\
&+ \sum_{k=1}^{\infty} c^{-k} \frac{\mathrm{i}m}{2\hbar} \sum_{n=1}^{\infty} (-1)^n \frac{1}{n} [\partial_t \operatorname{tr}(\eta g^{-1}_{(k,n)})] \psi \\
&+ \sum_{k=1}^{\infty} c^{-k} \frac{1}{2} \sum_{n=1}^{\infty} (-1)^n \frac{1}{n} [\partial_a \operatorname{tr}(\eta g^{-1}_{(k,n)})] \delta^{ab} \partial_b \psi + \sum_{k=1}^{\infty} c^{-k} (\partial_a g^{ab}_{(k)}) \partial_b \psi \\
&+ \sum_{k=1}^{\infty} c^{-k} g^{ab}_{(k)} \partial_a \partial_b \psi \\
&- \sum_{k=0}^{\infty} c^{-k} \frac{m^2}{\hbar^2} g^{00}_{(k+2)} \psi - \sum_{k=0}^{\infty} c^{-k} \frac{\mathrm{i}m}{\hbar} (\partial_a g^{0a}_{(k+1)}) \psi - \sum_{k=0}^{\infty} c^{-k} \frac{2\mathrm{i}m}{\hbar} g^{0a}_{(k+1)} \partial_a \psi \\
&+ \frac{2\mathrm{i}m}{\hbar} \partial_t \psi + \Delta \psi
\end{aligned} \tag{3.4.23}$$

Inserting the expansion $\psi = \sum_{k=0}^{\infty} c^{-k} a_k$ and using the Cauchy product formula, this is equivalent to

$$
\begin{aligned}
0 = & \sum_{k=5}^{\infty} c^{-k} \frac{1}{2} \sum_{l+m+\tilde{k}=k-2} \sum_{n=1}^{\infty} (-1)^n \frac{1}{n} g^{00}_{(m)} [\partial_t \operatorname{tr}(\eta g^{-1}_{(l,n)})] \, \partial_t a_{\tilde{k}} \\
& + \sum_{k=4}^{\infty} c^{-k} \sum_{l+\tilde{k}=k-2} (\partial_t g^{00}_{(l)}) \, \partial_t a_{\tilde{k}} + \sum_{k=4}^{\infty} c^{-k} \sum_{l+\tilde{k}=k-2} g^{00}_{(l)} \partial_t^2 a_{\tilde{k}} \\
& - \sum_{k=3}^{\infty} c^{-k} \frac{im}{2\hbar} \sum_{l+m+\tilde{k}=k} \sum_{n=1}^{\infty} (-1)^n \frac{1}{n} g^{00}_{(m)} [\partial_t \operatorname{tr}(\eta g^{-1}_{(l,n)})] a_{\tilde{k}} \\
& + \sum_{k=3}^{\infty} c^{-k} \frac{1}{2} \sum_{l+m+\tilde{k}=k-1} \sum_{n=1}^{\infty} (-1)^n \frac{1}{n} g^{0a}_{(m)} \Big([\partial_t \operatorname{tr}(\eta g^{-1}_{(l,n)})] \, \partial_a a_{\tilde{k}} + [\partial_a \operatorname{tr}(\eta g^{-1}_{(l,n)})] \, \partial_t a_{\tilde{k}} \Big) \\
& - \sum_{k=3}^{\infty} c^{-k} \frac{1}{2} \sum_{l+\tilde{k}=k-2} \sum_{n=1}^{\infty} (-1)^n \frac{1}{n} [\partial_t \operatorname{tr}(\eta g^{-1}_{(l,n)})] \, \partial_t a_{\tilde{k}} \\
& - \sum_{k=2}^{\infty} c^{-k} \frac{im}{\hbar} \sum_{l+\tilde{k}=k} (\partial_t g^{00}_{(l)}) a_{\tilde{k}} - \sum_{k=2}^{\infty} c^{-k} \frac{2im}{\hbar} \sum_{l+\tilde{k}=k} g^{00}_{(l)} \partial_t a_{\tilde{k}} \\
& + \sum_{k=2}^{\infty} c^{-k} \frac{1}{2} \sum_{l+m+\tilde{k}=k} \sum_{n=1}^{\infty} (-1)^n \frac{1}{n} g^{ab}_{(m)} [\partial_a \operatorname{tr}(\eta g^{-1}_{(l,n)})] \, \partial_b a_{\tilde{k}} \\
& + \sum_{k=2}^{\infty} c^{-k} \sum_{l+\tilde{k}=k-1} \Big((\partial_t g^{0a}_{(l)}) \, \partial_a a_{\tilde{k}} + (\partial_a g^{0a}_{(l)}) \, \partial_t a_{\tilde{k}} \Big) + \sum_{k=2}^{\infty} c^{-k} \, 2 \sum_{l+\tilde{k}=k-1} g^{0a}_{(l)} \partial_t \partial_a a_{\tilde{k}} \\
& - \sum_{k=2}^{\infty} c^{-k} \partial_t^2 a_{k-2} - \sum_{k=1}^{\infty} c^{-k} \frac{im}{2\hbar} \sum_{l+m+\tilde{k}=k+1} \sum_{n=1}^{\infty} (-1)^n \frac{1}{n} g^{0a}_{(m)} [\partial_a \operatorname{tr}(\eta g^{-1}_{(l,n)})] a_{\tilde{k}} \\
& + \sum_{k=1}^{\infty} c^{-k} \frac{im}{2\hbar} \sum_{l+\tilde{k}=k} \sum_{n=1}^{\infty} (-1)^n \frac{1}{n} [\partial_t \operatorname{tr}(\eta g^{-1}_{(l,n)})] a_{\tilde{k}} \\
& + \sum_{k=1}^{\infty} c^{-k} \frac{1}{2} \sum_{l+\tilde{k}=k} \sum_{n=1}^{\infty} (-1)^n \frac{1}{n} [\partial_a \operatorname{tr}(\eta g^{-1}_{(l,n)})] \delta^{ab} \partial_b a_{\tilde{k}} + \sum_{k=1}^{\infty} c^{-k} \sum_{l+\tilde{k}=k} (\partial_a g^{ab}_{(l)}) \partial_b a_{\tilde{k}} \\
& + \sum_{k=1}^{\infty} c^{-k} \sum_{l+\tilde{k}=k} g^{ab}_{(l)} \partial_a \partial_b a_{\tilde{k}} - \sum_{k=0}^{\infty} c^{-k} \frac{m^2}{\hbar^2} \sum_{l+\tilde{k}=k+2} g^{00}_{(l)} a_{\tilde{k}} \\
& - \sum_{k=0}^{\infty} c^{-k} \frac{im}{\hbar} \sum_{l+\tilde{k}=k+1} (\partial_a g^{0a}_{(l)}) a_{\tilde{k}} - \sum_{k=0}^{\infty} c^{-k} \frac{2im}{\hbar} \sum_{l+\tilde{k}=k+1} g^{0a}_{(l)} \partial_a a_{\tilde{k}} \\
& + \sum_{k=0}^{\infty} c^{-k} \frac{2im}{\hbar} \partial_t a_k + \sum_{k=0}^{\infty} c^{-k} \Delta a_k \, ,
\end{aligned}
\tag{3.4.24}
$$

where in sums like $\sum_{l+m+\tilde{k}=k}$, l and m are ≥ 1 as before, but $\tilde{k}$ is ≥ 0.

Using the fully expanded (3.4.24), we can obtain equations for the a_k, order by order, which can then be combined into a Schrödinger equation for ψ: at order c^0, we have

$$0 = \left(-\frac{m^2}{\hbar^2} g^{00}_{(2)} - \frac{\mathrm{i}m}{\hbar} (\partial_a g^{0a}_{(1)}) - \frac{2\mathrm{i}m}{\hbar} g^{0a}_{(1)} \partial_a + \frac{2\mathrm{i}m}{\hbar} \partial_t + \Delta \right) a_0 \,, \tag{3.4.25}$$

i.e. the Schrödinger equation

$$\mathrm{i}\hbar \partial_t a_0 = \left(-\frac{\hbar^2}{2m} \Delta + \frac{\mathrm{i}\hbar}{2} (\partial_a g^{0a}_{(1)}) + \mathrm{i}\hbar g^{0a}_{(1)} \partial_a + \frac{m}{2} g^{00}_{(2)} \right) a_0 \,. \tag{3.4.26}$$

By the relation $\psi = a_0 + \mathrm{O}(c^{-1})$, this also gives a Schrödinger equation for ψ in 0^{th} order in c^{-1}.

At order c^{-1}, (3.4.24) yields the following Schrödinger-like equation for a_1 with correction terms involving a_0:

$$\begin{aligned} \mathrm{i}\hbar \partial_t a_1 = {} & \left(-\frac{\hbar^2}{2m} \Delta + \frac{\mathrm{i}\hbar}{2} (\partial_a g^{0a}_{(1)}) + \mathrm{i}\hbar g^{0a}_{(1)} \partial_a + \frac{m}{2} g^{00}_{(2)} \right) a_1 \\ & + \bigg(- \frac{\mathrm{i}\hbar}{4} g^{0a}_{(1)} [\partial_a \operatorname{tr}(\eta g^{-1}_{(1)})] + \frac{\mathrm{i}\hbar}{4} [\partial_t \operatorname{tr}(\eta g^{-1}_{(1)})] + \frac{\hbar^2}{4m} [\partial_a \operatorname{tr}(\eta g^{-1}_{(1)})] \delta^{ab} \partial_b \\ & - \frac{\hbar^2}{2m} (\partial_a g^{ab}_{(1)}) \partial_b - \frac{\hbar^2}{2m} g^{ab}_{(1)} \partial_a \partial_b + \frac{m}{2} g^{00}_{(3)} + \frac{\mathrm{i}\hbar}{2} (\partial_a g^{0a}_{(2)}) + \mathrm{i}\hbar g^{0a}_{(2)} \partial_a \bigg) a_0 \end{aligned} \tag{3.4.27}$$

Using $\psi = a_0 + c^{-1} a_1 + \mathrm{O}(c^{-2})$, we can combine (3.4.27) with (3.4.26) into a Schrödinger equation for ψ up to order c^{-1}:

$$\begin{aligned} \mathrm{i}\hbar \partial_t \psi = \bigg[& - \frac{\hbar^2}{2m} \Delta + \frac{\mathrm{i}\hbar}{2} (\partial_a g^{0a}_{(1)}) + \mathrm{i}\hbar g^{0a}_{(1)} \partial_a + \frac{m}{2} g^{00}_{(2)} + c^{-1} \bigg(- \frac{\mathrm{i}\hbar}{4} g^{0a}_{(1)} [\partial_a \operatorname{tr}(\eta g^{-1}_{(1)})] \\ & + \frac{\mathrm{i}\hbar}{4} [\partial_t \operatorname{tr}(\eta g^{-1}_{(1)})] + \frac{\hbar^2}{4m} [\partial_a \operatorname{tr}(\eta g^{-1}_{(1)})] \delta^{ab} \partial_b - \frac{\hbar^2}{2m} (\partial_a g^{ab}_{(1)}) \partial_b - \frac{\hbar^2}{2m} g^{ab}_{(1)} \partial_a \partial_b \\ & + \frac{m}{2} g^{00}_{(3)} + \frac{\mathrm{i}\hbar}{2} (\partial_a g^{0a}_{(2)}) + \mathrm{i}\hbar g^{0a}_{(2)} \partial_a \bigg) + \mathrm{O}(c^{-2}) \bigg] \psi =: H\psi \end{aligned} \tag{3.4.28}$$

Continuing this process of evaluating (3.4.24), we can, in principle, get Schrödinger equations for ψ to arbitrary order in c^{-1}, i.e. obtain the Hamiltonian in the Schrödinger form of the positive frequency Klein–Gordon equation to arbitrary order in c^{-1}.

However, when considering higher orders, a difficulty arises: the Schrödinger-like equations for a_k begin to involve time derivatives of the lower order functions a_l, so we have to re-use the derived equations for the a_l in order to get a true Schrödinger equation for ψ (with a purely 'spatial' Hamiltonian, i.e. not involving any time derivatives) – i.e. the process becomes recursive. As far as concrete calculations up to some finite order are concerned, this is merely a computational obstacle; but for a general analysis of the expansion method this poses a bigger problem, since no general closed form can be easily obtained. This motivated the study of the Klein–Gordon equation as a quadratic equation for the time derivative operator, leading to the 'momentum expansion' method described in section 3.5.

3.4.2. Transformation to 'flat' scalar product and comparison with canonical quantisation

To transform the Hamiltonian obtained in (3.4.28) from the representation of the Hilbert space with the Klein–Gordon inner product (3.3.2) to the 'flat' scalar product (3.2.6) in order to compare it to the result from canonical quantisation, we note that for two positive frequency solutions $\Psi_{\text{KG}} = \exp(-\mathrm{i}mc^2 t/\hbar)\psi$ and $\Phi_{\text{KG}} = \exp(-\mathrm{i}mc^2 t/\hbar)\varphi$, the Klein–Gordon inner product is given by

$$\begin{aligned}
\langle \Psi_{\text{KG}}, \Phi_{\text{KG}} \rangle_{\text{KG}} &= \mathrm{i}\hbar c \int \mathrm{d}^3\boldsymbol{x}\, \sqrt{{}^{(3)}g}\, g^{0\nu} [(\partial_\nu \overline{\Psi_{\text{KG}}})\Phi_{\text{KG}} - \overline{\Psi_{\text{KG}}}(\partial_\nu \Phi_{\text{KG}})] \frac{1}{\sqrt{-g^{00}}} \\
&= \int \mathrm{d}^3\boldsymbol{x}\, \sqrt{{}^{(3)}g} \left(\sqrt{-g^{00}} \left[2mc^2 \overline{\psi}\varphi + \overline{(H\psi)}\varphi + \overline{\psi}(H\varphi) \right] \right. \\
&\qquad \left. + \mathrm{i}\hbar c \frac{g^{0a}}{\sqrt{-g^{00}}} \left[\overline{(\partial_a \psi)}\varphi - \overline{\psi}(\partial_a \varphi) \right] \right),
\end{aligned} \tag{3.4.29}$$

where we used our adapted coordinates and chose $\Sigma = \{t = \text{const.}\}$ in the general form (3.3.2) of the Klein–Gordon inner product.

Using $\sqrt{-g^{00}} = 1 + \mathrm{O}(c^{-2})$, $g^{0a}(-g^{00})^{-1/2} = \mathrm{O}(c^{-1})$, and $H = \mathrm{O}(c^0)$, we get

$$\frac{1}{2mc^2} \langle \Psi_{\text{KG}}, \Phi_{\text{KG}} \rangle_{\text{KG}} = \int \mathrm{d}^3\boldsymbol{x}\, \sqrt{{}^{(3)}g}\, [\overline{\psi}\varphi + \mathrm{O}(c^{-2})]. \tag{3.4.30}$$

For this to equal the 'flat' scalar product $\int \mathrm{d}^3\boldsymbol{x}\, \overline{\psi_{\mathrm{f}}}\, \varphi_{\mathrm{f}}$, we see that the 'flat wavefunction' has to have the form $\psi_{\mathrm{f}} = {}^{(3)}g^{1/4}\, \psi + \mathrm{O}(c^{-2})$ and therefore evolves according to the Schrödinger equation $\mathrm{i}\hbar\partial_t \psi_{\mathrm{f}} = H_{\mathrm{f}}\, \psi_{\mathrm{f}}$ with the 'flat Hamiltonian'

$$H_{\mathrm{f}} = \mathrm{i}\hbar \left(\partial_t {}^{(3)}g^{1/4} \right) {}^{(3)}g^{-1/4} + {}^{(3)}g^{1/4}\, H \left({}^{(3)}g^{-1/4} \cdot \right) + \mathrm{O}(c^{-2}). \tag{3.4.31}$$

Using[5] ${}^{(3)}g^{1/4} = 1 - c^{-1}\frac{1}{4}\operatorname{tr}(\eta g^{-1}_{(1)}) + \mathrm{O}(c^{-2})$ and noting that conjugation with a multiplication operator leaves multiplication operators invariant, we obtain

$$\begin{aligned}
H_{\mathrm{f}} &= -\mathrm{i}\hbar c^{-1}\frac{1}{4}[\partial_t \operatorname{tr}(\eta g^{-1}_{(1)})] + H - c^{-1}\frac{\hbar^2}{8m}[\Delta, \operatorname{tr}(\eta g^{-1}_{(1)})] \\
&\quad + c^{-1}\frac{\mathrm{i}\hbar}{4} g^{0a}_{(1)}[\partial_a, \operatorname{tr}(\eta g^{-1}_{(1)})] + \mathrm{O}(c^{-2}) \\
&= -\mathrm{i}\hbar c^{-1}\frac{1}{4}[\partial_t \operatorname{tr}(\eta g^{-1}_{(1)})] + H - c^{-1}\frac{\hbar^2}{8m}\left([\Delta \operatorname{tr}(\eta g^{-1}_{(1)})] + 2[\partial_a \operatorname{tr}(\eta g^{-1}_{(1)})]\delta^{ab}\partial_b\right) \\
&\quad + c^{-1}\frac{\mathrm{i}\hbar}{4} g^{0a}_{(1)}[\partial_a \operatorname{tr}(\eta g^{-1}_{(1)})] + \mathrm{O}(c^{-2}) \\
&= -\frac{\hbar^2}{2m}\Delta + \frac{\mathrm{i}\hbar}{2}(\partial_a g^{0a}_{(1)}) + \mathrm{i}\hbar g^{0a}_{(1)}\partial_a + \frac{m}{2}g^{00}_{(2)} + c^{-1}\bigg(- \frac{\hbar^2}{2m}(\partial_a g^{ab}_{(1)})\,\partial_b - \frac{\hbar^2}{2m}g^{ab}_{(1)}\partial_a\partial_b \\
&\quad + \frac{m}{2}g^{00}_{(3)} + \frac{\mathrm{i}\hbar}{2}(\partial_a g^{0a}_{(2)}) + \mathrm{i}\hbar g^{0a}_{(2)}\partial_a - \frac{\hbar^2}{8m}[\Delta \operatorname{tr}(\eta g^{-1}_{(1)})]\bigg) + \mathrm{O}(c^{-2}) \\
&= -\frac{\hbar^2}{2m}\Delta - \frac{1}{2}\left\{g^{0a}_{(1)}, -\mathrm{i}\hbar\partial_a\right\} + \frac{m}{2}g^{00}_{(2)} + c^{-1}\bigg(\frac{1}{2m}(-\mathrm{i}\hbar)\partial_a\Big(g^{ab}_{(1)}(-\mathrm{i}\hbar)\partial_b\,\cdot\Big) \\
&\quad + \frac{m}{2}g^{00}_{(3)} - \frac{1}{2}\left\{g^{0a}_{(2)}, -\mathrm{i}\hbar\partial_a\right\} - \frac{\hbar^2}{8m}[\Delta \operatorname{tr}(\eta g^{-1}_{(1)})]\bigg) + \mathrm{O}(c^{-2}),
\end{aligned} \tag{3.4.32}$$

where $\{A, B\} = AB + BA$ denotes the anticommutator. This is the Hamiltonian appearing in the 'flat' Schrödinger form of the positive frequency Klein–Gordon equation up to order c^{-1}, obtained by the WKB-like approximation in a general metric.

For comparison of this result with the canonical quantisation scheme, we have to subtract the rest energy mc^2 from the classical Hamiltonian of equation (3.2.2), corresponding to the phase factor separated off the Klein–Gordon field, and expand it in c^{-1}, yielding

$$\begin{aligned}
H_{\mathrm{class}} &= \frac{1}{\sqrt{-g^{00}}}c\left[m^2c^2 + \left(g^{ab} - \frac{1}{g^{00}}g^{0a}g^{0b}\right)p_a p_b\right]^{1/2} - mc^2 + \frac{c}{g^{00}}g^{0a}p_a \\
&= \frac{m}{2}g^{00}_{(2)} + \frac{\boldsymbol{p}^2}{2m} - g^{0a}_{(1)}p_a + c^{-1}\left(\frac{m}{2}g^{00}_{(3)} + g^{ab}_{(1)}\frac{p_a p_b}{2m} - g^{0a}_{(2)}p_a\right) + \mathrm{O}(c^{-2}).
\end{aligned} \tag{3.4.33}$$

[5]The metric determinant satisfies $g^{-1} = -1 - c^{-1}\operatorname{tr}(\eta g^{-1}_{(1)}) + \mathrm{O}(c^{-2})$. Using the well-known identity ${}^{(3)}g = g^{00}g$ for a $3+1$ decomposed metric, this gives ${}^{(3)}g = g^{00}g = [-1 + \mathrm{O}(c^{-2})][-1 + c^{-1}\operatorname{tr}(\eta g^{-1}_{(1)}) + \mathrm{O}(c^{-2})] = 1 - c^{-1}\operatorname{tr}(\eta g^{-1}_{(1)}) + \mathrm{O}(c^{-2})$.

Comparing this with (3.4.32), we see that by 'canonical quantisation' of this classical Hamiltonian using the rule '$p_i \to -\mathrm{i}\hbar\partial_i$', we can reproduce, using a specific ordering scheme, all terms appearing in the WKB expansion, apart from $-\frac{\hbar^2}{8mc}[\Delta\,\mathrm{tr}(\eta g_{(1)}^{-1})]$. For this last term to arise by naive canonical quantisation, consisting only of symmetrising according to some ordering scheme and replacing momenta by operators, in the classical Hamiltonian there would have to be a term proportional to $\frac{p^2}{mc}\,\mathrm{tr}(\eta g_{(1)}^{-1}) = \frac{p^2}{mc}\delta_{ab} g_{(1)}^{ab}$, which is not the case.

As the most simple non-trivial example, for the 'Newtonian' metric with line element

$$\mathrm{d}s^2 = -\left(1 + 2\frac{\phi}{c^2}\right) c^2 \mathrm{d}t^2 + \mathrm{d}\boldsymbol{x}^2 + \mathrm{O}(c^{-2}), \tag{3.4.34}$$

the inverse metric has components

$$(g^{\mu\nu}) = \begin{pmatrix} -1 + 2\frac{\phi}{c^2} + \mathrm{O}(c^{-4}) & \mathrm{O}(c^{-3}) \\ \mathrm{O}(c^{-3}) & \mathbb{1} + \mathrm{O}(c^{-2}) \end{pmatrix}, \tag{3.4.35}$$

leading to the quantum Hamiltonian $H = -\frac{\hbar^2}{2m}\Delta + m\phi + \mathrm{O}(c^{-2})$ in both schemes, i.e. just the standard Hamiltonian with Newtonian potential.

The occurrence of an extra term in a geometrically motivated quantum theory which one cannot arrive at by naive canonical quantisation is reminiscent of the occurrence of a 'quantum-mechanical potential' term in the Hamiltonian found by DeWitt in his 1952 treatment of quantum motion in a curved space [DeW52]: by demanding the (free part of the) Hamiltonian to be given by $H^{\mathrm{DeWitt}} = -\frac{\hbar^2}{2m}{}^{(3)}\Delta_{\mathrm{LB}}$ in terms of the spatial Laplace–Beltrami operator ${}^{(3)}\Delta_{\mathrm{LB}}$ (induced by the *physical* spatial metric ${}^{(3)}g$, not the background flat one), it turns out to have the form $H^{\mathrm{DeWitt}} = \frac{1}{2m}\hat{p}_a\,{}^{(3)}g^{ab}\,\hat{p}_b + \hbar^2 Q$ of a sum of a naively canonically quantised kinetic term[6] and the quantum-mechanical potential[7] $\hbar^2 Q = \frac{\hbar^2}{2m}{}^{(3)}g^{-1/4}\partial_a({}^{(3)}g^{ab}\partial_b{}^{(3)}g^{1/4})$.

[6]Note that DeWitt uses the 'geometric' scalar product (3.2.4), not the 'flat' one.

[7]Using the form

$$\begin{aligned} -\hbar^{2\,(3)}\Delta_{\mathrm{LB}} &= -\hbar^2 \frac{1}{\sqrt{{}^{(3)}g}}\partial_a\left(\sqrt{{}^{(3)}g}\,{}^{(3)}g^{ab}\partial_b\,\cdot\right) \\ &= {}^{(3)}g^{-1/4}\,\hat{p}_a\,{}^{(3)}g^{1/2}\,{}^{(3)}g^{ab}\,\hat{p}_b\,{}^{(3)}g^{-1/4} \end{aligned} \tag{3.4.36}$$

of the Laplace–Beltrami operator in terms of the momentum operator (3.2.5), it can be expressed as

$$-\hbar^{2\,(3)}\Delta_{\mathrm{LB}} = \hat{p}_a\,{}^{(3)}g^{ab}\,\hat{p}_b - {}^{(3)}g^{-1/4}[\hat{p}_a, {}^{(3)}g^{ab}[\hat{p}_b, {}^{(3)}g^{1/4}]], \tag{3.4.37}$$

giving the above expression for the quantum-mechanical potential.

In fact, for our metric (2.4.4), in lowest order in c^{-1} the quantum-mechanical potential is given by $\hbar^2 Q = -\frac{\hbar^2}{8mc}\Delta(\delta_{ab}g^{ab}_{(1)}) + \mathrm{O}(c^{-2}) = -\frac{\hbar^2}{8mc}[\Delta\,\mathrm{tr}(\eta g^{-1}_{(1)})] + \mathrm{O}(c^{-2})$, thus reproducing the additional term arising in the WKB method. This apparent connection of our WKB-like expansion to the three-dimensional 'spatial' geometry seems interesting, but further investigation in this direction goes beyond the scope of this thesis, since in this post-Newtonian context, the explicit comparison to the Newtonian limit – which also includes flat space – is the specific subject of interest.

Note that one could argue that DeWitt's Hamiltonian *can* be arrived at by canonical quantisation in some sense, since the Laplace–Beltrami operator can be written as $-\hbar^2\,{}^{(3)}\Delta_{\mathrm{LB}} = {}^{(3)}g^{-1/4}\,\hat{p}_a\,{}^{(3)}g^{1/2}\,{}^{(3)}g^{ab}\,\hat{p}_b\,{}^{(3)}g^{-1/4}$ in terms of the momentum operator (3.2.5) corresponding to the 'geometric' scalar product (3.2.4) which was used by DeWitt. However, such a 'clever rewriting' of the Newtonian kinetic term in the classical Hamiltonian as $\frac{1}{2m}{}^{(3)}g^{ab}p_a p_b = \frac{1}{2m}{}^{(3)}g^{-1/4}\,p_a\,{}^{(3)}g^{1/2}\,{}^{(3)}g^{ab}\,p_b\,{}^{(3)}g^{-1/4}$ before replacing momenta by operators involves more than just choosing some symmetrised operator ordering, and thus is not part of what we called 'canonical quantisation' above.

3.4.3. The Eddington–Robertson PPN metric as an explicit example

We now will apply the WKB-like expansion method to the Eddington–Robertson parametrised post-Newtonian metric as given by (2.5.1), (2.5.2).

Inserting the metric components, the equations arising for the coefficient functions a_0, a_1 from (3.4.24) at orders c^0, c^{-1} are simply the Schrödinger equations

$$\mathrm{i}\hbar\partial_t a_i = \left(-\frac{\hbar^2}{2m}\Delta + m\phi\right)a_i, \quad i = 0,1. \tag{3.4.38}$$

At orders c^{-2}, c^{-3}, we get – again for $i = 0,1$ –

$$\begin{aligned}
0 = \Bigg[&-\frac{\mathrm{i}m}{\hbar}(\partial_t g^{00}_{(2)}) - \frac{2\mathrm{i}m}{\hbar}g^{00}_{(2)}\partial_t - \partial_t^2 + \frac{\mathrm{i}m}{2\hbar}\left(-[\partial_t\,\mathrm{tr}(\eta g^{-1}_{(2)})] + \frac{1}{2}[\partial_t\,\mathrm{tr}(\eta\,\underbrace{g^{-1}_{(2,2)}}_{=g^{-1}_{(1)}\eta g^{-1}_{(1)}=0})]\right)\\
&+\frac{1}{2}\left(-[\partial_a\,\mathrm{tr}(\eta g^{-1}_{(2)})]\delta^{ab}\partial_b + \frac{1}{2}[\partial_a\,\mathrm{tr}(\eta g^{-1}_{(2,2)})]\delta^{ab}\partial_b\right)\\
&+(\partial_a g^{ab}_{(2)})\,\partial_b + g^{ab}_{(2)}\partial_a\partial_b - \frac{m^2}{\hbar^2}g^{00}_{(4)}\Bigg]a_i + \left(-\frac{m^2}{\hbar^2}g^{00}_{(2)} + \frac{2\mathrm{i}m}{\hbar}\partial_t + \Delta\right)a_{i+2}\\
= \Bigg(&-\frac{4\mathrm{i}m}{\hbar}\phi\partial_t - \partial_t^2 - \frac{\mathrm{i}m}{\hbar}(3\gamma+1)(\partial_t\phi) - (\gamma-1)(\partial_a\phi)\delta^{ab}\partial_b\\
&+2\gamma\phi\Delta - \frac{m^2}{\hbar^2}(2\beta-4)\phi^2\Bigg)a_i + \left(-\frac{2m^2}{\hbar^2}\phi + \frac{2\mathrm{i}m}{\hbar}\partial_t + \Delta\right)a_{i+2}\,,
\end{aligned} \tag{3.4.39}$$

or equivalently the Schrödinger-like equations

$$\begin{aligned}\mathrm{i}\hbar\partial_t a_{i+2} = \left(-\frac{\hbar^2}{2m}\Delta + m\phi\right) a_{i+2} + \bigg(2\mathrm{i}\hbar\phi\partial_t + \frac{\hbar^2}{2m}\partial_t^2 + \frac{\mathrm{i}\hbar}{2}(3\gamma+1)(\partial_t\phi)\\ + \frac{\hbar^2}{2m}(\gamma-1)(\partial_a\phi)\delta^{ab}\partial_b - \frac{\hbar^2}{m}\gamma\phi\Delta + \frac{m}{2}(2\beta-4)\phi^2\bigg) a_i\end{aligned} \tag{3.4.40}$$

for a_2, a_3. Using the Schrödinger equation (3.4.38) for a_0, a_1, we have

$$\begin{aligned}\frac{\hbar^2}{2m}\partial_t^2 a_i &= -\frac{\mathrm{i}\hbar}{2m}\partial_t\left(-\frac{\hbar^2}{2m}\Delta + m\phi\right) a_i = -\frac{\mathrm{i}\hbar}{2}(\partial_t\phi)a_i - \frac{1}{2m}\left(-\frac{\hbar^2}{2m}\Delta + m\phi\right)\mathrm{i}\hbar\partial_t a_i\\ &= -\frac{\mathrm{i}\hbar}{2}(\partial_t\phi)a_i - \frac{1}{2m}\left(-\frac{\hbar^2}{2m}\Delta + m\phi\right)^2 a_i\\ &= -\frac{\mathrm{i}\hbar}{2}(\partial_t\phi)a_i - \frac{\hbar^4}{8m^3}\Delta\Delta a_i + \frac{\hbar^2}{4m}\Delta(\phi a_i) + \frac{\hbar^2}{4m}\phi\Delta a_i - \frac{m}{2}\phi^2 a_i\\ &= -\frac{\mathrm{i}\hbar}{2}(\partial_t\phi)a_i - \frac{\hbar^4}{8m^3}\Delta\Delta a_i + \frac{\hbar^2}{4m}(\Delta\phi)a_i + \frac{\hbar^2}{2m}(\partial_a\phi)\delta^{ab}\partial_b a_i + \frac{\hbar^2}{2m}\phi\Delta a_i - \frac{m}{2}\phi^2 a_i\,,\end{aligned} \tag{3.4.41}$$

and thus the equation for a_2, a_3 becomes

$$\begin{aligned}\mathrm{i}\hbar\partial_t a_{i+2} = \left(-\frac{\hbar^2}{2m}\Delta + m\phi\right) a_{i+2} + \bigg(- \frac{\hbar^4}{8m^3}\Delta\Delta + \frac{\hbar^2}{4m}(\Delta\phi) + \frac{3\mathrm{i}\hbar}{2}\gamma(\partial_t\phi)\\ + \frac{\hbar^2}{2m}\gamma(\partial_a\phi)\delta^{ab}\partial_b - \frac{\hbar^2}{2m}(2\gamma+1)\phi\Delta + \frac{m}{2}(2\beta-1)\phi^2\bigg) a_i\,.\end{aligned} \tag{3.4.42}$$

At higher orders, the coefficients in the expanded Klein–Gordon equation (3.4.24) are undetermined, since the metric components are undetermined.

Combining the equations (3.4.38) for a_0, a_1 and (3.4.42) for a_2, a_3, the Hamiltonian in the Schrödinger equation $\mathrm{i}\hbar\partial_t\psi = H\psi$ for the 'wavefunction' (i.e. phase-shifted positive-frequency Klein–Gordon field) ψ reads

$$\begin{aligned}H = -\frac{\hbar^2}{2m}\Delta + m\phi + \frac{1}{c^2}\bigg(- \frac{\hbar^4}{8m^3}\Delta\Delta + \frac{\hbar^2}{4m}(\Delta\phi) + \frac{3\mathrm{i}\hbar}{2}\gamma(\partial_t\phi)\\ + \frac{\hbar^2}{2m}\gamma(\partial_a\phi)\delta^{ab}\partial_b - \frac{\hbar^2}{2m}(2\gamma+1)\phi\Delta + \frac{m}{2}(2\beta-1)\phi^2\bigg) + \mathrm{O}(c^{-4}),\end{aligned} \tag{3.4.43}$$

reproducing, up to notational differences and the fact that we did not consider coupling to an electromagnetic field, the result of Lämmerzahl [Läm95, eq. (8)].

To transform to the flat scalar product, we note that in our metric and using this Hamiltonian, the Klein–Gordon inner product (3.4.29) is given by

$$\frac{1}{2mc^2}\langle\Psi_{\mathrm{KG}},\Phi_{\mathrm{KG}}\rangle_{\mathrm{KG}} = \int \mathrm{d}^3\boldsymbol{x}\,\sqrt{{}^{(3)}g}\,\left(\overline{\psi}\varphi - \frac{\hbar^2}{2m^2c^2}\overline{\psi}\Delta\varphi + \mathrm{O}(c^{-4})\right). \tag{3.4.44}$$

Note that in the brackets, we did not need to expand any further since the factor $\sqrt{{}^{(3)}g}$ is only determined up to $\mathrm{O}(c^{-4})$ by the metric (2.5.1). For the expression (3.4.44) to equal the flat scalar product $\int \mathrm{d}^3\boldsymbol{x}\,\overline{\psi_\mathrm{f}}\,\varphi_\mathrm{f}$, the flat wavefunction has to have the form $\psi_\mathrm{f} = \left(1 - \frac{\hbar^2}{2m^2c^2}\Delta\right)^{1/2} {}^{(3)}g^{1/4}\,\psi + \mathrm{O}(c^{-4})$ (note that $\frac{1}{c^2}\Delta$ commutes with ${}^{(3)}g$ up to higher-order terms), resulting in the flat Hamiltonian

$$\begin{aligned} H_\mathrm{f} = {} & \mathrm{i}\hbar\left(\partial_t {}^{(3)}g^{1/4}\right) {}^{(3)}g^{-1/4} \\ & + \left(1 - \frac{\hbar^2}{2m^2c^2}\Delta\right)^{1/2} {}^{(3)}g^{1/4}\,H\,{}^{(3)}g^{-1/4}\left(1 - \frac{\hbar^2}{2m^2c^2}\Delta\right)^{-1/2} + \mathrm{O}(c^{-4}). \end{aligned} \tag{3.4.45}$$

Using ${}^{(3)}g^{1/4} = 1 - \frac{3}{2}\gamma\frac{\phi}{c^2} + \mathrm{O}(c^{-4})$ and $\left(1 - \frac{\hbar^2}{2m^2c^2}\Delta\right)^{1/2} = 1 - \frac{\hbar^2}{4m^2c^2}\Delta + \mathrm{O}(c^{-4})$, this yields

$$\begin{aligned} H_\mathrm{f} &= -\mathrm{i}\hbar\left(\partial_t\frac{3}{2}\gamma\frac{\phi}{c^2}\right) + H + \left[-\frac{3}{2}\gamma\frac{\phi}{c^2}, -\frac{\hbar^2}{2m}\Delta\right] + \left[-\frac{\hbar^2}{4m^2c^2}\Delta, m\phi\right] + \mathrm{O}(c^{-4}) \\ &= -\frac{3\mathrm{i}\hbar}{2c^2}\gamma(\partial_t\phi) + H - \frac{\hbar^2}{4mc^2}(3\gamma+1)[\Delta,\phi] + \mathrm{O}(c^{-4}) \\ &= -\frac{3\mathrm{i}\hbar}{2c^2}\gamma(\partial_t\phi) + H - \frac{\hbar^2}{4mc^2}(3\gamma+1)((\Delta\phi) + 2(\partial_a\phi)\delta^{ab}\partial_b) + \mathrm{O}(c^{-4}) \\ &= -\frac{\hbar^2}{2m}\Delta + m\phi + \frac{1}{c^2}\bigg(-\frac{\hbar^4}{8m^3}\Delta\Delta - \frac{3\hbar^2}{4m}\gamma(\Delta\phi) \\ &\qquad - \frac{\hbar^2}{2m}(2\gamma+1)(\partial_a\phi)\delta^{ab}\partial_b - \frac{\hbar^2}{2m}(2\gamma+1)\phi\Delta + \frac{m}{2}(2\beta-1)\phi^2\bigg) + \mathrm{O}(c^{-4}), \end{aligned} \tag{3.4.46}$$

reproducing the flat Hamiltonian of Lämmerzahl [Läm95, eq. (16)].

In comparison, the classical Hamiltonian (minus the rest energy) expands to

$$\begin{aligned} H_\mathrm{class} &= \frac{1}{\sqrt{-g^{00}}}c\left[m^2c^2 + \left(g^{ab} - \frac{1}{g^{00}}g^{0a}g^{0b}\right)p_a p_b\right]^{1/2} - mc^2 + \frac{c}{g^{00}}g^{0a}p_b \\ &= \frac{\boldsymbol{p}^2}{2m} + m\phi + c^{-2}\left(-\frac{(\boldsymbol{p}^2)^2}{8m^3} + \frac{m\phi^2}{2}(2\beta-1) + \frac{\phi}{2m}(2\gamma+1)\boldsymbol{p}^2\right) + \mathrm{O}(c^{-4}). \end{aligned} \tag{3.4.47}$$

By canonical quantisation of this, we cannot reproduce the Hamiltonian obtained from the WKB expansion in the case of a general γ, but just for some special choices of γ, depending on the ordering scheme: for example, in the anticommutator ordering scheme, we would quantise the classical function $\phi \boldsymbol{p}^2$ as

$$\frac{1}{2}\{-\hbar^2\Delta, \phi\} = -\frac{\hbar^2}{2}(\Delta\phi) - \hbar^2(\partial_a\phi)\delta^{ab}\partial_b - \hbar^2\phi\Delta\,, \tag{3.4.48}$$

reproducing the WKB Hamiltonian in the case of $\gamma = 1$; but when quantising it as $-\hbar^2\delta^{ab}\partial_a(\phi\partial_b\,\cdot) = -\hbar^2(\partial_a\phi)\delta^{ab}\partial_b - \hbar^2\phi\Delta$, this would lead to agreement with the WKB Hamiltonian for $\gamma = 0$. Note however that this difference concerns a term proportional to $\Delta\phi$, the Laplacian of the Newtonian potential. By the Newtonian gravitational field equation, this term is (in lowest order) proportional to the mass density generating the gravitational field. Thus it is irrelevant in physical situations concerning the outside of the generating matter distribution, for example in quantum-optical experiments in the gravitational field of the earth taking place outside of the earth. Nevertheless, this example shows that the way in which PPN parameters enter a quantum description delicately depends on the quantisation method.

3.5. General comparison of the two methods by momentum expansion

We will now describe a method by which general statements about similarities and differences between the two approaches explained above can be made in the case of stationary spacetimes, without any post-Newtonian expansion in c^{-1}. Instead, we consider 'potential' terms and terms linear, quadratic, … in momentum, i.e. we perform a (formal) expansion in momenta. Of course, this also amounts to somewhat of a post-Newtonian expansion – although just relating to the particle momentum/velocity, not the gravitational field *per se*.

3.5.1. The Klein–Gordon equation as a quadratic equation for the Hamiltonian

We assume a *stationary* physical spacetime such that the background time evolution vector field[8] $u = \partial_t$ is (a constant multiple of) the stationarity Killing field, i.e. $\partial_t g_{\mu\nu} = 0$.

[8] In fact, for the 'momentum expansion' to be developed in the following we do not need to expand the physical metric in any way, and thus we do not need a background metric to define a notion of 'absence of gravity'. Nevertheless, we need a notion of 'space' – but this could also be given by something else than the orthogonal complement of the stationarity field with respect to a background

The coordinate expression for the d'Alembert operator on functions is thus

$$\begin{aligned}\Box f &= \frac{1}{\sqrt{-g}}\partial_\mu(\sqrt{-g}g^{\mu\nu}\partial_\nu f)\\ &= \frac{1}{\sqrt{-g}}(\partial_\mu\sqrt{-g})g^{\mu\nu}\partial_\nu f + (\partial_\mu g^{\mu\nu})\partial_\nu f + g^{\mu\nu}\partial_\mu\partial_\nu f\\ &= \frac{1}{2g}(\partial_a g)g^{a\nu}\partial_\nu f + (\partial_a g^{a\nu})\partial_\nu f + g^{\mu\nu}\partial_\mu\partial_\nu f. \end{aligned} \tag{3.5.1}$$

Hence, the minimally coupled Klein–Gordon equation reads

$$\begin{aligned}0 &= \left(\Box - \frac{m^2c^2}{\hbar^2}\right)\Psi\\ &= \frac{1}{c}\frac{1}{2g}(\partial_a g)g^{0a}\partial_t\Psi + \frac{1}{2g}(\partial_a g)g^{ab}\partial_b\Psi + \frac{1}{c}(\partial_a g^{0a})\,\partial_t\Psi + (\partial_a g^{ab})\partial_b\Psi\\ &\quad + \frac{1}{c^2}g^{00}\partial_t^2\Psi + \frac{2}{c}g^{0a}\partial_a\partial_t\Psi + g^{ab}\partial_a\partial_b\Psi - \frac{m^2c^2}{\hbar^2}\Psi. \end{aligned} \tag{3.5.2}$$

This means that the space of solutions of the Klein–Gordon equation is the kernel of $\mathcal{P}(\mathrm{i}\hbar\partial_t)$, where for an operator A acting on the functions on the spacetime, $\mathcal{P}(A)$ is the following operator:

$$\begin{aligned}\mathcal{P}(A) = &-\frac{\mathrm{i}}{\hbar c}\frac{1}{2g}(\partial_a g)g^{0a}A + \frac{1}{2g}(\partial_a g)g^{ab}\partial_b - \frac{\mathrm{i}}{\hbar c}(\partial_a g^{0a})A + (\partial_a g^{ab})\partial_b\\ &- \frac{1}{\hbar^2c^2}g^{00}A^2 - \frac{2\mathrm{i}}{\hbar c}g^{0a}\partial_a \circ A + g^{ab}\partial_a\partial_b - \frac{m^2c^2}{\hbar^2} \end{aligned} \tag{3.5.3}$$

Thus, wanting to write the Klein–Gordon equation in the form of a Schrödinger equation $\mathrm{i}\hbar\partial_t\Psi = H\Psi$ (and thus restricting to the solutions of the Klein–Gordon equation for which this is possible), we see that this can be achieved by demanding the Hamiltonian H to be a solution of the quadratic operator equation

$$0 = \mathcal{P}(H) \tag{3.5.4}$$

and be composed only of spatial derivative operators and coefficients of the metric, not involving any time derivatives: stationarity of the metric then implies $[\partial_t, H] = 0$, such that the Schrödinger equation yields $(\mathrm{i}\hbar\partial_t)^2\Psi = \mathrm{i}\hbar\partial_t H\Psi = H\mathrm{i}\hbar\partial_t\Psi = H^2\Psi$, leading to

metric. In any case, our approach based on a background metric leads to a decomposition as needed in an easy and well-defined geometric way.

$\mathcal{P}(\mathrm{i}\hbar\partial_t)\Psi = \mathcal{P}(H)\Psi = 0$ by (3.5.4); i.e. every solution of the Schrödinger equation is also a solution of the Klein–Gordon equation.

In the following, we will solve equation (3.5.4) by expanding H as a formal power series in spatial derivative operators, i.e. momentum operators. The two possible solutions we will obtain for H correspond to positive and negative frequency solutions of the Klein–Gordon equation, respectively.

3.5.2. Momentum expansion and first-order solution

We expand H as $H = H_{(0)} + H_{(1)} + \mathrm{O}(\partial_a^2)$, where $H_{(k)}$ includes all terms involving k spatial derivative operators. Using this notation, the lowest order term of (3.5.4), involving no spatial derivatives, reads

$$0 = -\frac{1}{\hbar^2 c^2} g^{00} H_{(0)}^2 - \frac{m^2 c^2}{\hbar^2}, \tag{3.5.5}$$

giving

$$H_{(0)} = \frac{mc^2}{\sqrt{-g^{00}}} \tag{3.5.6}$$

where we choose the positive square root since we are interested in positive frequency solutions of the Klein–Gordon equation.

At order ∂_a^1, equation (3.5.4) gives

$$\begin{aligned} 0 = &-\frac{\mathrm{i}}{\hbar c}\frac{1}{2g}(\partial_a g) g^{0a} H_{(0)} - \frac{\mathrm{i}}{\hbar c}(\partial_a g^{0a}) H_{(0)} \\ &- \frac{1}{\hbar^2 c^2} g^{00}(2H_{(0)}H_{(1)} + [H_{(1)}, H_{(0)}]) - \frac{2\mathrm{i}}{\hbar c} g^{0a}\partial_a \circ H_{(0)}\ . \end{aligned} \tag{3.5.7}$$

Writing $H_{(1)} = H_{(1,M)} + H^a_{(N,C)}\partial_a$ where $H_{(1,M)}$ is a *m*ultiplication operator (involving one spatial differentiation of some function) and $H^a_{(N,C)}$ are *c*oefficient functions *n*ot involving any differentiations, we have $[H_{(1)}, H_{(0)}] = [H^a_{(1,C)}\partial_a, H_{(0)}] = H^a_{(1,C)}(\partial_a H_{(0)})$. Thus, the equation reads

$$\begin{aligned} 0 = &-\frac{\mathrm{i}}{\hbar c}\frac{1}{2g}(\partial_a g) g^{0a} H_{(0)} - \frac{\mathrm{i}}{\hbar c}(\partial_a g^{0a}) H_{(0)} - \frac{2g^{00}}{\hbar^2 c^2} H_{(0)} H_{(1)} \\ &- \frac{g^{00}}{\hbar^2 c^2} H^a_{(1,C)}(\partial_a H_{(0)}) - \frac{2\mathrm{i}}{\hbar c} g^{0a}(\partial_a H_{(0)}) - \frac{2\mathrm{i}}{\hbar c} g^{0a} H_{(0)}\partial_a\ . \end{aligned} \tag{3.5.8}$$

The right-hand side now has two different components: a multiplication operator and an operator differentiating the function it acts upon. We demand that these components vanish independently. The 'differentiating part' of (3.5.8) is

$$0 = -\frac{2g^{00}}{\hbar^2 c^2} H_{(0)} H^a_{(1,C)} \partial_a - \frac{2\mathrm{i}}{\hbar c} g^{0a} H_{(0)} \partial_a \, , \tag{3.5.9}$$

or equivalently

$$H^a_{(1,C)} = -\mathrm{i}\hbar c \frac{g^{0a}}{g^{00}} \, . \tag{3.5.10}$$

Using this, the multiplication operator part of (3.5.8) reads

$$0 = -\frac{\mathrm{i}}{\hbar c} \frac{1}{2g} (\partial_a g) g^{0a} H_{(0)} - \frac{\mathrm{i}}{\hbar c} (\partial_a g^{0a}) H_{(0)} - \frac{2g^{00}}{\hbar^2 c^2} H_{(0)} H_{(1,M)} - \frac{\mathrm{i}}{\hbar c} g^{0a} (\partial_a H_{(0)}), \tag{3.5.11}$$

giving

$$H_{(1,M)} = -\frac{\mathrm{i}\hbar c}{4g^{00} g} (\partial_a g) g^{0a} - \frac{\mathrm{i}\hbar c}{2g^{00}} (\partial_a g^{0a}) - \frac{\mathrm{i}\hbar c}{2g^{00}} g^{0a} \frac{1}{H_{(0)}} (\partial_a H_{(0)}). \tag{3.5.12}$$

Since $\frac{1}{H_{(0)}} (\partial_a H_{(0)}) = \sqrt{-g^{00}} \, \partial_a \frac{1}{\sqrt{-g^{00}}} = \frac{g^{00}}{2} \partial_a \frac{1}{g^{00}}$, equations (3.5.6), (3.5.10) and (3.5.12) together yield the result

$$H = \frac{mc^2}{\sqrt{-g^{00}}} - \frac{\mathrm{i}\hbar c}{4g^{00} g} (\partial_a g) g^{0a} - \frac{\mathrm{i}\hbar c}{2g^{00}} (\partial_a g^{0a}) - \frac{\mathrm{i}\hbar c}{4} g^{0a} \left(\partial_a \frac{1}{g^{00}} \right) - \mathrm{i}\hbar c \frac{g^{0a}}{g^{00}} \partial_a + \mathrm{O}(\partial_a^2) \tag{3.5.13}$$

for the Hamiltonian in the Schrödinger form

$$\mathrm{i}\hbar \partial_t \Psi = H\Psi \tag{3.5.14}$$

of the positive frequency Klein–Gordon equation, at first order in momenta.

3.5.3. Transformation to 'flat' scalar product and comparison with canonical quantisation

To transform this Hamiltonian to the 'flat' scalar product, we note that for two positive frequency solutions Ψ and Φ, the Klein–Gordon inner product is given by

$$\begin{aligned}
\langle \Psi, \Phi \rangle_{\mathrm{KG}} &= \mathrm{i}\hbar c \int \mathrm{d}^3 \boldsymbol{x} \sqrt{{}^{(3)}g} \, g^{0\nu} [(\partial_\nu \overline{\Psi}) \Phi - \overline{\Psi} (\partial_\nu \Phi)] \frac{1}{\sqrt{-g^{00}}} \\
&= \int \mathrm{d}^3 \boldsymbol{x} \sqrt{{}^{(3)}g} \Bigg(\sqrt{-g^{00}} \left[\overline{(H\Psi)} \Phi + \overline{\Psi} (H\Phi) \right] \\
&\qquad + \mathrm{i}\hbar c \frac{g^{0a}}{\sqrt{-g^{00}}} \left[\overline{(\partial_a \Psi)} \Phi - \overline{\Psi} (\partial_a \Phi) \right] \Bigg) \\
\text{(using (3.5.13))} \quad &= \int \mathrm{d}^3 \boldsymbol{x} \sqrt{{}^{(3)}g} \, 2mc^2 \, \overline{\Psi} \Phi + \mathrm{O}(\partial_a^2).
\end{aligned} \tag{3.5.15}$$

For this to equal the 'flat' scalar product $\int \mathrm{d}^3\boldsymbol{x}\,\overline{\Psi_\mathrm{f}}\,\Phi_\mathrm{f}$, we see that the 'flat wavefunction' has to have the form $\Psi_\mathrm{f} = \sqrt{2mc^2}\,{}^{(3)}g^{1/4}\,\Psi + \mathrm{O}(\partial_a^2)$, and therefore evolves according to the Schrödinger equation $\mathrm{i}\hbar\partial_t\Psi_\mathrm{f} = H_\mathrm{f}\Psi_\mathrm{f}$ with the 'flat Hamiltonian'

$$H_\mathrm{f} = {}^{(3)}g^{1/4}\,H\left({}^{(3)}g^{-1/4}\cdot\right) + \mathrm{O}(\partial_a^2). \tag{3.5.16}$$

For calculating H_f from H, we note that conjugating with a multiplication operator leaves multiplication operators invariant and that

$$\begin{aligned} {}^{(3)}g^{1/4}\,\partial_a\left({}^{(3)}g^{-1/4}\cdot\right) &= \partial_a - \frac{1}{4}\left[\partial_a \ln\left({}^{(3)}g\right)\right] \\ &= \partial_a - \frac{1}{4}\left[\partial_a \ln\left(g^{00}g\right)\right] \\ &= \partial_a - \frac{1}{4}\frac{1}{g}(\partial_a g) - \frac{1}{4}\frac{1}{g^{00}}\left(\partial_a g^{00}\right), \end{aligned} \tag{3.5.17}$$

yielding the final result

$$\begin{aligned} H_\mathrm{f} &= \frac{mc^2}{\sqrt{-g^{00}}} - \frac{\mathrm{i}\hbar c}{4g^{00}g}(\partial_a g)g^{0a} - \frac{\mathrm{i}\hbar c}{2g^{00}}\left(\partial_a g^{0a}\right) - \frac{\mathrm{i}\hbar c}{4}g^{0a}\left(\partial_a \frac{1}{g^{00}}\right) \\ &\quad - \mathrm{i}\hbar c\frac{g^{0a}}{g^{00}}\left(\partial_a - \frac{1}{4g}(\partial_a g) - \frac{1}{4g^{00}}\left(\partial_a g^{00}\right)\right) + \mathrm{O}(\partial_a^2) \\ &= \frac{mc^2}{\sqrt{-g^{00}}} - \frac{\mathrm{i}\hbar c}{2}\left(\partial_a \frac{g^{0a}}{g^{00}}\right) - \mathrm{i}\hbar c\frac{g^{0a}}{g^{00}}\partial_a + \mathrm{O}(\partial_a^2) \\ &= \frac{mc^2}{\sqrt{-g^{00}}} + c\frac{1}{2}\left\{\frac{g^{0a}}{g^{00}}, -\mathrm{i}\hbar\partial_a\right\} + \mathrm{O}(\partial_a^2). \end{aligned} \tag{3.5.18}$$

Looking at the momentum expansion of the classical Hamiltonian

$$\begin{aligned} H_\text{class} &= \frac{1}{\sqrt{-g^{00}}}c\left[m^2c^2 + \left(g^{ab} - \frac{1}{g^{00}}g^{0a}g^{0b}\right)p_a p_b\right]^{1/2} + \frac{c}{g^{00}}g^{0a}p_a \\ &= \frac{mc^2}{\sqrt{-g^{00}}} + \frac{c}{g^{00}}g^{0a}p_a + \mathrm{O}(p_a^2), \end{aligned} \tag{3.5.19}$$

we see that 'canonical quantisation' of this Hamiltonian will lead to the same 'potential term' and to the same term linear in momentum as did the Klein–Gordon equation, regardless of the adopted ordering scheme. The reason for this is that for terms of linear order in momentum, any ordering scheme leads to 'anticommutator quantisation', as is easily shown:

Any general canonically quantised, arbitrarily symmetrised operator of linear order in momentum is the sum of terms of the form $\hat{A} = \frac{1}{2}(f\bar{p}_a h + h\bar{p}_a f)$, where f, h are real-valued functions of position (here identified with the corresponding self-adjoint multiplication operators). The classical phase space function corresponding to $\hat{A}$ is $A = \frac{1}{2}(f p_a h + h p_a f) = f h p_a$. Rewriting $\hat{A}$ as

$$\begin{aligned}
\hat{A} &= \frac{1}{2}(f\bar{p}_a h + h\bar{p}_a f) = \frac{1}{2}\big(\bar{p}_a f h + [f, \bar{p}_a]h + h f\bar{p}_a + h[\bar{p}_a, f]\big) \\
&= \frac{1}{2}\big(\bar{p}_a f h + (\mathrm{i}\hbar\partial_a f)h + h f\bar{p}_a - h(\mathrm{i}\hbar\partial_a f)\big) = \frac{1}{2}(\bar{p}_a f h + h f\bar{p}_a) \\
&= \frac{1}{2}\{fh, \bar{p}_a\},
\end{aligned} \tag{3.5.20}$$

we thus see that it arises from A by 'anticommutator quantisation', as desired.

We thus have shown that in stationary post-Newtonian spacetimes, the Hamiltonians obtained by naive canonical quantisation of free particle motion and by formally expanding the Klein–Gordon equation agree to linear order in momentum. In particular, this means that the lowest-order coupling to gravitomagnetic fields agrees in both methods.

4. Post-Newtonian Hamiltonian description of an atom in a weak gravitational field

In this chapter, we extend the systematic calculation of an 'approximately relativistic', i.e. first order post-Newtonian, Hamiltonian for centre of mass and internal dynamics of an electromagnetically bound two-particle system by Sonnleitner and Barnett [SB18] to the case including a weak post-Newtonian gravitational background field, described by the Eddington–Robertson PPN metric. Starting from a properly relativistic description of the situation, this approach allows to systematically *derive* the coupling of the model system to gravity, instead of 'guessing' it by means of classical notions of 'relativistic effects'.

This chapter is based on material that has been published in [SG19b]. However, here we significantly extend the published results by dropping the approximating assumption of constant gravitational potential over the extent of the system. We also clarify a small inconsistency that was present in the treatment of the non-gravitational case by Sonnleitner and Barnett in [SB18], as well as in our published article [SG19b].

4.1. Introduction

Motivated by inconsistencies in the usual approximative Galilei-relativistic description of quantum-optical interactions of atoms with light, which by an *ad hoc* semi-classical argumentation are easily seen to be possibly resolved in a special-relativistic description, Sonnleitner and Barnett have developed in [SB18] a fully systematic derivation of an 'approximately relativistic' Hamiltonian describing a simple atom in an external electromagnetic field. It is the purpose of this chapter to extend this so as to also include gravity approximately, more precisely a post-Newtonian gravitational field as described by the Eddington–Robertson PPN metric. As discussed in the introduction, such a generalisation is, apart from its conceptual value, of immediate interest for describing and devising quantum-optical experiments in gravitational fields, e.g. in atom interferometry.

The greatest value of Sonnleitner and Barnett's basing their whole calculation in [SB18] on a properly relativistic treatment of the situation (an atom interacting with an external electromagnetic field) can be seen in allowing a systematic derivation of a complete description without any *ad hoc* assumptions. In the end, the first-order post-Newtonian Hamiltonian they obtained could *then* be used to interpret aspects of the situation in terms of classical 'relativistic corrections'. For example, the 'centre of mass' part of the final Hamiltonian has the form of a single-particle kinetic Hamiltonian, where the rôle of the rest mass of this particle is played by the total mass-energy of the atom, i.e. the sum of the rest masses of the constituent particles and the internal atomic energy divided by c^2. Thus, the computation in [SB18] explicitly shows that this physically intuitive picture of a 'composite particle', suggested by mass–energy equivalence, can, in fact, be derived in a controlled and systematic approximation scheme, rather than merely made plausible from semi-intuitive physical considerations.

As will be shown by our calculations, a similar interpretation is possible for the situation including external gravitational fields: when expressing the final Hamiltonian using the physical spacetime metric, an intuitive 'composite point particle' picture including the 'mass defect' due to mass–energy equivalence will again be available for the centre of mass dynamics. This lends justification based on detailed calculations within systematic approximation schemes to some of the naiver approaches that are based on *a priori* assumptions concerning the gravity–matter coupling.

In section 4.2, we set up the background for our calculations: after describing the physical system under consideration, we will give a somewhat detailed exposition of the method of computation in [SB18], in which we will also address an inconsistency of the original approach. Then we will discuss how our geometric post-Newtonian expansion framework introduced in chapter 2 allows us to develop our gravitational calculation in parallel to that from [SB18].

In the following, we will compute in detail the 'gravitational corrections' to the calculation by Sonnleitner and Barnett [SB18] arising from the presence of the gravitational field. Section 4.3 will deal with the coupling of the gravitational field to the kinetic terms of the particles only, ignoring couplings of the gravitational to the electromagnetic field.

In section 4.4, we will then compute the Lagrangian of the electromagnetic field in the presence of the gravitational field. This allows us to compute the total Hamiltonian describing the atomic system in section 4.5.1, by repeating the calculation from section 4.3 while including the 'gravitational corrections' to electromagnetism as obtained in section 4.4. The resulting Hamiltonian will then be interpreted in terms of the physical spacetime metric and compared to earlier results in the remainder of section 4.5.

In sections 4.3 and 4.5.1, we will very closely follow the calculation from and presentation in [SB18]. For the reader's convenience, we have reproduced all the relevant formulae from [SB18] that are used in our calculation in section 4.2.1, in which we describe Sonnleitner and Barnett's work. We use the original numbering, prepended with '[SB18].', so for example ([SB18].25f) refers to equation (25f) of [SB18]. As some of the equations from [SB18] contain minor errors (mostly sign errors), we here give corrected versions. The corresponding equation numbers are marked with a star, e.g. ([SB18].12⋆).

A calculation using methods very similar to those of [SB18] including external gravitational fields was performed by Marzlin already in 1995 [Mar95][1]; but unlike Sonnleitner and Barnett in [SB18] or our calculation in the following, Marzlin did not perform a full first-order post-Newtonian expansion and instead focused on the electric dipole coupling only.

4.2. A composite system in external electromagnetic and gravitational fields

We consider a simple system consisting of two particles without spin, with respective electric charges e_1, e_2, masses m_1, m_2, and spatial positions $\boldsymbol{r}_1, \boldsymbol{r}_2$. For simplicity we assume the charges to be equal and opposite, i.e. $e_2 = -e_1 =: e$. In what follows, we will take into account their mutual electromagnetic interaction, but neglect their mutual gravitational interaction. This two-particle system, which we will sometimes refer to as 'atom', will be placed in an external electromagnetic field, which we will take into account, as well as an external gravitational field, which we will also take into account. It is our inclusion of the latter that extends the previous study [SB18].

4.2.1. External electromagnetic fields – the work of Sonnleitner and Barnett

In [SB18], Sonnleitner and Barnett describe a systematic method to obtain an 'approximately relativistic' quantum Hamiltonian for a system as described above interacting with an external electromagnetic field, where 'approximately relativistic' refers to the inclusion of lowest order post-Newtonian correction terms, i.e. of order c^{-2}. Their work was motivated by their own observation [STB17; BS18] that the electromagnetic interaction of a decaying atom, which in QED follows an intrinsically special-relativistic symmetry (i.e. Poincaré invariance), will give rise to unnaturally looking friction-like terms that seem to contradict the relativity principle (which, of course, they don't) if interpreted in a 'non-relativistic' (i.e. Galilei-invariant) setting of ordinary quantum mechanics. Their correct conclusion in [SB18] was that this confusion can be altogether avoided by replacing this 'hotchpotch' (their wording, see last line on p. 042106-9 of

[1] I am grateful to Alexander Friedrich for pointing out this reference to me.

[SB18]) of symmetry concepts by a systematic post-Newtonian derivation starting from a common, manifestly Poincaré-symmetric description.

As our development will closely follow theirs, we will now describe the strategy of [SB18] in some detail. In the course of this, we will also reproduce all formulae from [SB18] that will be used in the remainder of this chapter. We use the original numbering, prepended with '[SB18].'. For formulae containing errors in [SB18] (mostly sign errors), we give here a corrected version; the corrections are highlighted in red and the number is marked with a star. In addition to that, there is a conceptual inconsistency in the treatment in [SB18] that we will address below. This will necessitate some further (rather small) amendments to the equations, which will be marked in the same way as the other errors.

Sonnleitner and Barnett start with the classical Poincaré-invariant Lagrangian function describing two particles interacting with electromagnetic potentials[2]:

$$L = -\sum_{i=1,2} m_i c^2 \sqrt{1 - \dot{\boldsymbol{r}}_i^2/c^2} + \int \mathrm{d}^3\boldsymbol{x}\, (\boldsymbol{j} \cdot \boldsymbol{A}_{\text{tot.}} - \rho\phi_{\text{el.,tot.}}) + \frac{\varepsilon_0}{2} \int \mathrm{d}^3\boldsymbol{x}\, [(\partial_t \boldsymbol{A}_{\text{tot.}} + \boldsymbol{\nabla}\phi_{\text{el.,tot.}})^2 - c^2(\boldsymbol{\nabla} \times \boldsymbol{A}_{\text{tot.}})^2]. \qquad \text{([SB18].4)}$$

Note that we have changed the variable name of the total electric potential to $\phi_{\text{el.,tot.}}$ so as to avoid confusion with the Newtonian gravitational potential ϕ from the Eddington–Robertson PPN metric. $\boldsymbol{j}$ denotes the electric current density of the particles, and ρ the charge density.

Sonnleitner and Barnett then split the electromagnetic potentials into 'internal' (i.e. generated by the particles) and 'external' parts, employ the Coulomb gauge, and solve the Maxwell equations for the internal part in lowest order, expressing the solutions in terms of the particles' positions and velocities (see the solutions in ([SB18].A1) and ([SB18].A3) at the end of this section). The total vector potential, which is a transverse field (in the Helmholtz decomposition) due to the gauge condition, is split as $\boldsymbol{A}^{\perp}_{\text{tot.}} = \boldsymbol{A}^{\perp} + \boldsymbol{\mathcal{A}}^{\perp}$ where $\boldsymbol{A}^{\perp}$ denotes the external and $\boldsymbol{\mathcal{A}}^{\perp}$ the internal part. Due to the absence of external electric charges and the gauge condition, the external electric potential vanishes, such that $\phi_{\text{el.,tot.}} = \phi_{\text{el.}}$ is purely internal.

The idea is now to insert the solutions for the internal potentials into the Lagrangian ([SB18].4) and expand the kinetic terms for the particles, so as to obtain a post-Newtonian Lagrangian on which to base the further derivation. However, at this stage an inconsistency is introduced into the framework of [SB18], which we are now going to explain. Sonnleitner and Barnett want to keep the external vector potential

[2]In the absence of gravity, as this is the situation considered in [SB18].

$\boldsymbol{A}^{\perp}$ as a dynamical variable; as such, its equations of motion have to be the vacuum Maxwell equations (i.e. without any source term), while it still has to enter the equations of motion of the particles themselves. This is indeed the case for the Lagrangian which arises from directly inserting the internal potentials as obtained by solving the Maxwell equations: variation of the action given by this Lagrangian leads to Euler–Lagrange equations just as desired. This Lagrangian, however, contains second-order time derivatives of the particle positions, spoiling the application of conventional Hamiltonian formalism. This problem does not show up when following Sonnleitner and Barnett, since the problematic terms are related to formally diverging backreaction terms and are therefore disregarded from the Lagrangian in [SB18]. However, *this* last neglection is problematic if one keeps the external vector potential $\boldsymbol{A}^{\perp}$ as dynamical: the just-eliminated terms would have been the ones ensuring the vacuum Maxwell equations as equations of motion for the external potential – without them, the Lagrangian gives, again, the *sourced* Maxwell equations for the external potential, and the formalism becomes inconsistent. This inconsistency was not addressed in [SB18], and we were also not aware of it at the time of publication of our article [SG19b].

However, as it turns out, there is a very easy way to remedy this problem: we proceed almost exactly like Sonnleitner and Barnett did, the only difference being that we remove the external vector potential $\boldsymbol{A}^{\perp}$ from its role as dynamical degree of freedom, treating it as a given external field instead (satisfying the vacuum Maxwell equations). This way we can ensure the consistency of the equations of motion while still performing the internal–external field split[3]. The one point in Sonnleitner and Barnett's derivation where one might be questioning if it still works without the electromagnetic field being a dynamical variable, namely the PZW transformation, will turn out to still be applicable just fine when reinterpreted in the right way, as we will explain below. Note that although the external field is eliminated as a dynamical variable, when Legendre transforming the Lagrangian in order to go over to the Hamiltonian formalism, we are going to add a term corresponding to the external field to the resulting Hamiltonian, such as to stay as close as possible to the original work of [SB18], and to obtain the correct value for the energy, including the external field energy[4].

[3] By employing some form of perturbation theory on a given non-zero classical background, as is sometimes used in quantum optics, it is probably possible to render the split into internal and external fields consistent while still keeping *some* electromagnetic / photonic degrees of freedom as dynamical variables. However, I (the author) am not well enough acquainted with such techniques – I myself being, more or less, a classical relativist – and thus restrict to those parts of the argumentation which I am confident of. If such a perturbation-theoretic treatment is indeed possible, it should be easily applicable to the results we will derive below.

[4] And to make our results as easily amenable as possible to a potential perturbation-theoretic treatment / interpretation as alluded to in the previous footnote.

Inserting the internal potential solutions and expanding the kinetic terms for the particles to order c^{-2} (disregarding the rest energy term), as well as neglecting electromagnetic terms of order $\mathrm{O}(c^{-4})$ and dropping terms related to formally diverging backreaction terms, one arrives at the post-Newtonian Lagrangian

$$\begin{aligned} L(\boldsymbol{r}_1, \dot{\boldsymbol{r}}_1, \boldsymbol{r}_2, \dot{\boldsymbol{r}}_2) &= L_{\text{Darwin}}(\boldsymbol{r}_1, \dot{\boldsymbol{r}}_1, \boldsymbol{r}_2, \dot{\boldsymbol{r}}_2) + \frac{\varepsilon_0}{2} \int \mathrm{d}^3\boldsymbol{x} \, [(\partial_t \boldsymbol{A}^\perp)^2 \\ &\quad - c^2 (\boldsymbol{\nabla} \times \boldsymbol{A}^\perp)^2] + \int \mathrm{d}^3\boldsymbol{x} \, \boldsymbol{j} \cdot \boldsymbol{A}^\perp \,, \qquad \text{([SB18].8}\star) \\ L_{\text{Darwin}}(\boldsymbol{r}_1, \dot{\boldsymbol{r}}_1, \boldsymbol{r}_2, \dot{\boldsymbol{r}}_2) &= \frac{m_1 \dot{\boldsymbol{r}}_1^2}{2} + \frac{m_1 \dot{\boldsymbol{r}}_1^4}{8c^2} + \frac{m_2 \dot{\boldsymbol{r}}_2^2}{2} + \frac{m_2 \dot{\boldsymbol{r}}_2^4}{8c^2} \\ &\quad - \frac{1}{4\pi\varepsilon_0} \frac{e_1 e_2}{r} \left(1 - \frac{\dot{\boldsymbol{r}}_1 \cdot \dot{\boldsymbol{r}}_2}{2c^2}\right) + \frac{e_1 e_2}{4\pi\varepsilon_0} \frac{(\dot{\boldsymbol{r}}_1 \cdot \boldsymbol{r})(\dot{\boldsymbol{r}}_2 \cdot \boldsymbol{r})}{2r^3 c^2} \,, \qquad \text{([SB18].9)} \end{aligned}$$

where $\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$ and $r = |\boldsymbol{r}|$. Note that here, as explained above, $\boldsymbol{A}^\perp$ is treated as a given external field that appears in the Lagrangian, not a dynamical variable. L_{Darwin} is the famous Darwin Lagrangian [Dar20], involving 'correction terms' to the Coulomb potential arising from the internal atomic motion.

This classical Lagrangian is then Legendre transformed to obtain a classical Hamiltonian. As explained above, in order to get the correct value for the energy, including the external field energy, we add a term as one would obtain when Legrendre transforming also with respect to the external field, even though it is not a dynamical variable. We also use the notation $\boldsymbol{\Pi}^\perp = \varepsilon_0 \partial_t \boldsymbol{A}^\perp$ for the 'would-be canonical momentum' conjugate to the external field, but have to keep in mind that it is a fixed field, not a real momentum conjugate to any configuration variable. As would be the case for a 'true' electromagnetic canonical momentum, $-\boldsymbol{\Pi}^\perp/\varepsilon_0 = -\partial_t \boldsymbol{A}^\perp = \boldsymbol{E}^\perp$ is, physically speaking, the external electric field.

Keeping these caveats in mind, the classical Hamiltonian reads

$$\begin{aligned} H &= \frac{\bar{\boldsymbol{p}}_1^2}{2m_1} - \frac{\bar{\boldsymbol{p}}_1^4}{8m_1^3 c^2} + \frac{\bar{\boldsymbol{p}}_2^2}{2m_2} - \frac{\bar{\boldsymbol{p}}_2^4}{8m_2^3 c^2} + \frac{1}{4\pi\varepsilon_0} \frac{e_1 e_2}{r} \left(1 - \frac{\bar{\boldsymbol{p}}_1 \cdot \bar{\boldsymbol{p}}_2}{2m_1 m_2 c^2}\right) \\ &\quad - \frac{e_1 e_2}{4\pi\varepsilon_0} \frac{(\bar{\boldsymbol{p}}_1 \cdot \boldsymbol{r})(\bar{\boldsymbol{p}}_2 \cdot \boldsymbol{r})}{2r^3 c^2 m_1 m_2} + \frac{\varepsilon_0}{2} \int \mathrm{d}^3\boldsymbol{x} \, [(\boldsymbol{\Pi}^\perp/\varepsilon_0)^2 + c^2 (\boldsymbol{\nabla} \times \boldsymbol{A}^\perp)^2], \qquad \text{([SB18].12}\star) \end{aligned}$$

where $\bar{\boldsymbol{p}}_i = \boldsymbol{p}_i - e_i \boldsymbol{A}^\perp(\boldsymbol{r}_i)$ ($\star$).

This classical Hamiltonian is now canonically quantised to obtain a quantum Hamiltonian in what Sonnleitner and Barnett call the 'minimal coupling form'. They then perform a Power–Zienau–Woolley (PZW) unitary transformation [PZ59; Woo71; BL83] together with a multipolar expansion of the external field in order to transform the Hamiltonian into a so-called 'multipolar form'. The details of this, including the neccessary amendments due to $\boldsymbol{A}^\perp$ no longer being a dynamical field, are as follows.

The PZW transformation operator is

$$U = \mathrm{e}^{-\mathrm{i}\Lambda} = \exp\left[-\frac{\mathrm{i}}{\hbar}\int \mathrm{d}^3\boldsymbol{x}\,\boldsymbol{\mathcal{P}}(\boldsymbol{x},t)\cdot\boldsymbol{A}^{\perp}(\boldsymbol{x},t)\right], \tag{[SB18].14$\star$}$$

where $\boldsymbol{\mathcal{P}}$ is the polarisation field

$$\boldsymbol{\mathcal{P}}(\boldsymbol{x},t) = \sum_{i=1,2} e_i[\boldsymbol{r}_i(t)-\boldsymbol{R}(t)]\int_0^1 \mathrm{d}\lambda\,\delta\big(\boldsymbol{x}-\boldsymbol{R}(t)-\lambda[\boldsymbol{r}_i(t)-\boldsymbol{R}(t)]\big). \tag{[SB18].15}$$

The transformation amounts to the following change of canonical momenta:

$$\boldsymbol{p}_i \to U\boldsymbol{p}_i U^{\dagger} = \boldsymbol{p}_i + \hbar\boldsymbol{\nabla}_{\boldsymbol{r}_i}\Lambda \tag{[SB18].19a}$$

Since we treat the external field as non-dynamical, none of the variables corresponding to it change under the transformation. However, to reflect the change that *would* happen if $\boldsymbol{A}^{\perp}$ were still a dynamical field[5], we introduce the notation $\tilde{\boldsymbol{\Pi}}^{\perp} := \boldsymbol{\Pi}^{\perp} - \boldsymbol{\mathcal{P}}^{\perp}$ for the 'would-be canonical field momentum' after the PZW transformation, amounting to the change

$$\boldsymbol{\Pi}^{\perp}(\boldsymbol{x}) \to \tilde{\boldsymbol{\Pi}}^{\perp}(\boldsymbol{x}) + \boldsymbol{\mathcal{P}}^{\perp}(\boldsymbol{x}) \tag{[SB18].19b$\star$}$$

in the Hamiltonian. Physically, in line with the usual interpretation for the canonical field momentum after a PZW transformation [BL83], $-\tilde{\boldsymbol{\Pi}}^{\perp} = -\boldsymbol{\Pi}^{\perp} + \boldsymbol{\mathcal{P}}^{\perp}(\boldsymbol{x}) = \boldsymbol{D}^{\perp}$ is the electric displacement field. Note that in [SB18], the somewhat misleading notation $\boldsymbol{E}^{\perp}$ is used for the quantity '$-$(external field momentum after PZW trafo)$^{\perp}/\varepsilon_0$', as if it corresponded to an electric field proper.

In electric dipole approximation, i.e. expanding to first order in $\bar{\boldsymbol{r}}_i := \boldsymbol{r}_i - \boldsymbol{R}$, and using $\sum_{j=1,2} e_j = 0$, one finds (see [SB18] for details)

$$\hbar\boldsymbol{\nabla}_{\boldsymbol{r}_{1,2}}\Lambda \simeq e_{1,2}[\boldsymbol{A}^{\perp}(\boldsymbol{R}) + (\bar{\boldsymbol{r}}_{1,2}\cdot\boldsymbol{\nabla})\boldsymbol{A}^{\perp}(\boldsymbol{R})] + \frac{e_1\boldsymbol{r}_1 + e_2\boldsymbol{r}_2}{2}\times[\boldsymbol{\nabla}\times\boldsymbol{A}^{\perp}(\boldsymbol{R})]. \tag{[SB18].21$\star$}$$

Thus, under the PZW transformation and the dipole approximation the momenta transform as $\boldsymbol{p}_i - e_i\boldsymbol{A}(\boldsymbol{r}_i) \to \boldsymbol{p}_i + \boldsymbol{d}\times\boldsymbol{B}(\boldsymbol{R})/2$ ($\star$), where $\boldsymbol{d} = e_1\boldsymbol{r}_1 + e_2\boldsymbol{r}_2$ is the electric dipole moment.

Terms of the form

$$\frac{\boldsymbol{p}_i\cdot[\boldsymbol{d}\times\boldsymbol{B}(\boldsymbol{R})]}{m_i m_j c^2} \propto \frac{|\boldsymbol{p}_i|}{m_i c}\,\frac{|\boldsymbol{d}\cdot\boldsymbol{E}(\boldsymbol{R})|}{m_j c^2} \tag{[SB18].22}$$

are neglected, since the atom–light interaction energy is assumed much smaller than the internal atomic energy, which is in turn much smaller than the rest energies of the

[5] Again with the intent of staying as close as possible to the original work [SB18], and to allow a possible perturbation-theoretic reinterpretation.

particles. The multipolar Hamiltonian in electric dipole approximation is then

$$\begin{aligned} H_{[\text{mult}]} \simeq & \frac{[\boldsymbol{p}_1 + \frac{1}{2}\boldsymbol{d} \times \boldsymbol{B}(\boldsymbol{R})]^2}{2m_1} + \frac{[\boldsymbol{p}_2 + \frac{1}{2}\boldsymbol{d} \times \boldsymbol{B}(\boldsymbol{R})]^2}{2m_2} \\ & - \frac{e^2}{4\pi\varepsilon_0 r} + \frac{\varepsilon_0}{2}\int \mathrm{d}^3\boldsymbol{x}\, [(\tilde{\boldsymbol{\Pi}}^\perp + \boldsymbol{\mathcal{P}}_d^\perp)^2/\varepsilon_0^2 + c^2\boldsymbol{B}^2] \\ & - \frac{\boldsymbol{p}_1^4}{8m_1^3c^2} - \frac{\boldsymbol{p}_2^4}{8m_2^3c^2} + \frac{e^2}{16\pi\varepsilon_0 c^2 m_1 m_2} \\ & \times \left[\boldsymbol{p}_1 \cdot \frac{1}{r}\boldsymbol{p}_2 + (\boldsymbol{p}_1 \cdot \boldsymbol{r})\frac{1}{r^3}(\boldsymbol{r} \cdot \boldsymbol{p}_2) + (1 \leftrightarrow 2)\right], \end{aligned} \qquad \text{([SB18].23}\star\text{)}$$

where $\boldsymbol{\mathcal{P}}_d = +\boldsymbol{d}\,\delta(\boldsymbol{x} - \boldsymbol{R})$ ($\star$) is the polarisation in electric dipole approximation.

Then, introducing Newtonian centre of mass and relative coordinates $\boldsymbol{R}, \boldsymbol{r}$, and the corresponding canonical momenta $\boldsymbol{P}, \boldsymbol{p}_r$, Sonnleitner and Barnett arrive at what they call the centre of mass Hamiltonian:

$$H_{[\text{com}]} = H_\text{C} + H_\text{A} + H_\text{AL} + H_\text{L} + H_\text{X} \qquad \text{([SB18].25a)}$$

$$H_\text{C} = \frac{\boldsymbol{P}^2}{2M}\left[1 - \frac{\boldsymbol{P}^2}{4M^2c^2} - \frac{1}{Mc^2}\left(\frac{\boldsymbol{p}_r^2}{2\mu} - \frac{e^2}{4\pi\varepsilon_0 r}\right)\right] \qquad \text{([SB18].25b}\star\text{)}$$

$$\begin{aligned} H_\text{A} = & \frac{\boldsymbol{p}_r^2}{2\mu}\left(1 - \frac{m_1^3 + m_2^3}{M^3}\frac{\boldsymbol{p}_r^2}{4\mu^2c^2}\right) - \frac{e^2}{4\pi\varepsilon_0} \\ & \times \left[\frac{1}{r} + \frac{1}{2\mu Mc^2}\left(\boldsymbol{p}_r \cdot \frac{1}{r}\boldsymbol{p}_r + \boldsymbol{p}_r \cdot \boldsymbol{r}\frac{1}{r^3}\boldsymbol{r} \cdot \boldsymbol{p}_r\right)\right] \end{aligned} \qquad \text{([SB18].25c)}$$

$$\begin{aligned} H_\text{AL} = & -\boldsymbol{d} \cdot \frac{\boldsymbol{D}^\perp(\boldsymbol{R})}{\varepsilon_0} + \frac{1}{2M}\{\boldsymbol{P} \cdot [\boldsymbol{d} \times \boldsymbol{B}(\boldsymbol{R})] + \text{H.c.}\} \\ & - \frac{m_1 - m_2}{4m_1m_2}\{\boldsymbol{p}_r \cdot [\boldsymbol{d} \times \boldsymbol{B}(\boldsymbol{R})] + \text{H.c.}\} \\ & + \frac{1}{8\mu}(\boldsymbol{d} \times \boldsymbol{B}(\boldsymbol{R}))^2 + \frac{1}{2\varepsilon_0}\int \mathrm{d}^3\boldsymbol{x}\, \boldsymbol{\mathcal{P}}_d^{\perp\,2}(\boldsymbol{x}, t) \end{aligned} \qquad \text{([SB18].25d}\star\text{)}$$

$$H_\text{L} = \frac{\varepsilon_0}{2}\int \mathrm{d}^3\boldsymbol{x}\, [(\boldsymbol{D}^\perp/\varepsilon_0)^2 + c^2\boldsymbol{B}^2] \qquad \text{([SB18].25e}\star\text{)}$$

$$\begin{aligned} H_\text{X} = & -\frac{(\boldsymbol{P} \cdot \boldsymbol{p}_r)^2}{2M^2\mu c^2} + \frac{e^2}{4\pi\varepsilon_0 r}\frac{(\boldsymbol{P} \cdot \boldsymbol{r}/r)^2}{2M^2c^2} \\ & + \frac{m_1 - m_2}{2\mu M^2c^2}\left\{(\boldsymbol{P} \cdot \boldsymbol{p}_r)\boldsymbol{p}_r^2/\mu - \frac{e^2}{8\pi\varepsilon_0}\right. \\ & \left. \times \left[\frac{1}{r}\boldsymbol{P} \cdot \boldsymbol{p}_r + \frac{1}{r^3}(\boldsymbol{P} \cdot \boldsymbol{r})(\boldsymbol{r} \cdot \boldsymbol{p}_r) + \text{H.c.}\right]\right\} \end{aligned} \qquad \text{([SB18].25f)}$$

Note that the Hamiltonian has been expressed in a form in which the external field enters in terms of the magnetic field $\boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}^\perp$ and the electric displacement field

$\boldsymbol{D}^\perp = -\tilde{\boldsymbol{\Pi}}^\perp = -\varepsilon_0 \partial_t \boldsymbol{A}^\perp + \boldsymbol{\mathcal{P}}^\perp$ (which was, as mentioned above, a little misleadingly called $\varepsilon_0 \boldsymbol{E}^\perp$ in [SB18]). The Hamiltonian is split into terms that may be interpreted as describing the central motion of the atom (H_C), the internal atomic motion (H_A), the interaction between the atom and the external ('light') field (H_AL), and a term giving the external electromagnetic field energy (H_L), as well as 'cross terms' (H_X) coupling the relative degrees of freedom to the central momentum $\boldsymbol{P}$.

In order to eliminate this cross-term coupling, Sonnleitner and Barnett perform a final canonical transformation to new coordinates $\boldsymbol{Q}, \boldsymbol{q}$ and momenta $\boldsymbol{P}, \boldsymbol{p}$, which leaves the Hamiltonian unchanged up to terms of order c^{-4} except for elimination of the cross terms and the replacements $(\boldsymbol{R}, \boldsymbol{r}, \boldsymbol{p}_r) \to (\boldsymbol{Q}, \boldsymbol{q}, \boldsymbol{p})$. This canonical transformation reads as follows:

$$\begin{aligned} \boldsymbol{R} &= \boldsymbol{Q} + \frac{m_1 - m_2}{2M^2c^2}\left[\left(\frac{\boldsymbol{p}^2}{2\mu}\boldsymbol{q} + \text{H.c.}\right) - \frac{e^2}{4\pi\varepsilon_0 q}\boldsymbol{q}\right] \\ &\quad - \frac{1}{4M^2c^2}[(\boldsymbol{q}\cdot\boldsymbol{P})\boldsymbol{p} + (\boldsymbol{P}\cdot\boldsymbol{p})\boldsymbol{q} + \text{H.c.}] \qquad \text{([SB18].26a)} \\ \boldsymbol{r} &= \boldsymbol{q} + \frac{m_1 - m_2}{2\mu M^2c^2}[(\boldsymbol{q}\cdot\boldsymbol{P})\boldsymbol{p} + \text{H.c.}] - \frac{\boldsymbol{q}\cdot\boldsymbol{P}}{2M^2c^2}\boldsymbol{P} \qquad \text{([SB18].26b)} \\ \boldsymbol{p}_r &= \boldsymbol{p} + \frac{\boldsymbol{p}\cdot\boldsymbol{P}}{2M^2c^2}\boldsymbol{P} - \frac{m_1 - m_2}{2M^2c^2} \\ &\quad \times \left[\frac{\boldsymbol{p}^2}{\mu}\boldsymbol{P} - \frac{e^2}{4\pi\varepsilon_0}\left(\frac{1}{q}\boldsymbol{P} - \frac{1}{q^3}(\boldsymbol{P}\cdot\boldsymbol{q})\boldsymbol{q}\right)\right] \qquad \text{([SB18].26c)} \end{aligned}$$

Finally, the internal electromagnetic potentials to our order of approximation (thus in particular neglecting retardation), as obtained by solving the internal Maxwell equations, are as follows:

$$\begin{aligned} \phi_{\text{el.,ng}}(\boldsymbol{x}, t) &= \frac{1}{4\pi\varepsilon_0}\int \mathrm{d}^3x' \, \frac{\rho(\boldsymbol{x}', t)}{|\boldsymbol{x} - \boldsymbol{x}'|} \qquad \text{([SB18].A1)} \\ \boldsymbol{\mathcal{A}}^\perp_{\text{ng}}(\boldsymbol{x}, t) &\simeq \frac{1}{4\pi\varepsilon_0 c^2}\int \mathrm{d}^3x' \, \frac{\boldsymbol{j}(\boldsymbol{x}', t)}{|\boldsymbol{x} - \boldsymbol{x}'|} + \frac{1}{(4\pi)^2\varepsilon_0 c^2}\int \mathrm{d}^3x' \\ &\quad \times \int \mathrm{d}^3x'' \, \frac{\boldsymbol{x} - \boldsymbol{x}'}{|\boldsymbol{x} - \boldsymbol{x}'|^3} \, \frac{\boldsymbol{j}(\boldsymbol{x}'', t)\cdot(\boldsymbol{x}' - \boldsymbol{x}'')}{|\boldsymbol{x}' - \boldsymbol{x}''|^3} \\ &= \frac{1}{8\pi\varepsilon_0 c^2}\sum_{i=1,2} e_i \left\{\frac{\dot{\boldsymbol{r}}_i}{|\boldsymbol{x} - \boldsymbol{r}_i|} + \frac{(\boldsymbol{x} - \boldsymbol{r}_i)[\dot{\boldsymbol{r}}_i\cdot(\boldsymbol{x} - \boldsymbol{r}_i)]}{|\boldsymbol{x} - \boldsymbol{r}_i|^3}\right\} \qquad \text{([SB18].A3)} \end{aligned}$$

Here we have changed the variable names of the potentials to conform to our notation – in particular we added the suffix 'ng', standing for 'non-gravitational' – and expressed the magnetic potential in terms of ε_0 instead of $\mu_0 = 1/(\varepsilon_0 c^2)$.

4.2.2. Including weak external gravitational fields

As already stated above, our contribution in this chapter will consist in generalising the calculation of [SB18] to the case of the atom being situated in a weak external gravitational field in addition to the electromagnetic field already considered in [SB18]. Our aim is to likewise obtain an 'approximately relativistic', i.e. first-order post-Newtonian, Hamiltonian describing this situation. The gravitational field will be described by the Eddington–Robertson PPN metric as introduced in section 2.5.

Our post-Newtonian expansion scheme as laid out in chapter 2, based on the introduction of geometric background structures that give meaning to 'weak' gravitational fields and 'slow' velocities in the setting of a non-flat spacetime, provides the conceptual and computational basis which will allow us to implement the post-Newtonian expansion employed in [SB18] also in the gravitational case. This enables us to develop our calculation in great parallel with that of [SB18]: we use the 'flat' background structure to perform our computations, the benefit being the aimed-for direct comparison with [SB18]. In the course of our derivation, 'gravitational correction terms' to the non-gravitational formulae will show up. However, as already alluded to in section 2.2, it often is of great physical value to re-express the obtained results in terms of the physical metric g instead of the background metric η. For example, the results will contain geometric operations, like scalar products, which may be taken using either of the metric structures provided by the formalism. What may at first appear as a more or less complicated gravitational correction to the flat space result will often, in fact, turn out to be a simple and straightforward transcription of the latter into the proper physical metric, as one might have anticipated from some more or less naive working-version of the equivalence principle. Interpretational issues like this are well-known in the literature on gravitational couplings of quantum systems; see, e.g., [Mar95; Läm95]. For us, too, they will once more turn out to be relevant in connection with the total Hamiltonian in section 4.5. We will derive and interpret the relevant gravitational terms relative to the background structures (η, u) in order to keep the analogy with the computation in [SB18], but then we shall re-interpret the results in terms of the proper physical metric g in order to reveal their naturalness.

Since we are interested in a lowest-order post-Newtonian description, we will work up to (and including) terms of order c^{-2} and neglect higher order terms. In fact, corrections of higher order cannot be treated in a simple Hamiltonian formalism as employed here, without explicitly including the internal electromagnetic field degrees of freedom as dynamical variables: elimination of the internal field variables by solving Maxwell's equations will introduce retardation effects at higher orders, thus leading to an action that is non-local in time, spoiling the application of conventional Hamiltonian formalism.

4.3. Coupling the gravitational field to the particles

In this section we will work out the influence of the gravitational field when coupled to the kinetic terms of the particles only, ignoring its couplings to the electromagnetic field. The latter will be the subject of the following sections.

Starting from the Lagrangian for our atom in the *absence* of gravity and adding the 'gravitational corrections' to the kinetic terms of the particles, we will then repeat the calculation of [SB18] to obtain a quantum Hamiltonian in centre of mass coordinates.

4.3.1. The classical Hamiltonian

For a single free point particle with mass m and position $\boldsymbol{x}$, the classical kinetic Lagrangian (parametrising the worldline by coordinate time) in our metric (2.5.1) reads

$$\begin{aligned} L_{\text{point}} &= -mc^2\sqrt{-g_{\mu\nu}\dot{x}^\mu\dot{x}^\nu/c^2} \\ &= \frac{m\dot{\boldsymbol{x}}^2}{2}\left(1+\frac{\dot{\boldsymbol{x}}^2}{4c^2}\right) - mc^2 - m\phi\left(1+(2\beta-1)\frac{\phi}{2c^2}\right) - \frac{2\gamma+1}{2}\frac{m\phi}{c^2}\dot{\boldsymbol{x}}^2 + \mathrm{O}(c^{-4}). \end{aligned} \tag{4.3.1}$$

Now considering our two-particle system, the kinetic terms for the particles in gravity are given as the sum of two terms as in (4.3.1). These lowest-order 'gravitationally corrected' kinetic terms we include into the classical Lagrangian from ([SB18].4)[6], which described two particles interacting with an electromagnetic field in the *absence* of gravity.

Eliminating the internal electromagnetic fields literally as in the non-gravitational case, we arrive at the post-Newtonian classical Lagrangian

$$\begin{aligned} L_{\text{new}} = L &- m_1\phi(\boldsymbol{r}_1) - m_2\phi(\boldsymbol{r}_2) - \frac{2\gamma+1}{2}\frac{m_1\phi(\boldsymbol{r}_1)}{c^2}\dot{\boldsymbol{r}}_1^2 - \frac{2\gamma+1}{2}\frac{m_2\phi(\boldsymbol{r}_2)}{c^2}\dot{\boldsymbol{r}}_2^2 \\ &- (2\beta-1)\frac{m_1\phi(\boldsymbol{r}_1)^2}{2c^2} - (2\beta-1)\frac{m_2\phi(\boldsymbol{r}_2)^2}{2c^2} \end{aligned} \tag{4.3.2}$$

describing our electromagnetically bound two-particle system in the given external electromagnetic field. Here L is the final classical Lagrangian from ([SB18].8⋆) and ([SB18].9). Note that, as explained in section 4.2.1, for reasons of consistency, we view the external vector potential as a given background field, not as a dynamical variable.

Legendre transforming this Lagrangian with respect to the particle velocities $\dot{\boldsymbol{r}}_i$ and adding a term as one would obtain when Legrendre transforming also with respect to

[6] We remind the reader that all the equations from [SB18] that we refer to explicitly are reproduced in section 4.2.1.

the external electromagnetic vector potential (see section 4.2.1 before ([SB18].12⋆)), we obtain the total classical Hamiltonian

$$\begin{aligned} H_{\mathrm{new}} = H &+ m_1\phi(\boldsymbol{r}_1) + m_2\phi(\boldsymbol{r}_2) + \frac{2\gamma+1}{2m_1c^2}\phi(\boldsymbol{r}_1)\bar{\boldsymbol{p}}_1^2 + \frac{2\gamma+1}{2m_2c^2}\phi(\boldsymbol{r}_2)\bar{\boldsymbol{p}}_2^2 \\ &+ (2\beta-1)\frac{m_1\phi(\boldsymbol{r}_1)^2}{2c^2} + (2\beta-1)\frac{m_2\phi(\boldsymbol{r}_2)^2}{2c^2}. \end{aligned} \tag{4.3.3}$$

Here H is the classical Hamiltonian from ([SB18].12⋆) and $\bar{\boldsymbol{p}}_i = \boldsymbol{p}_i - e_i\boldsymbol{A}^{\perp}(\boldsymbol{r}_i)$ is the kinetic momentum. Note that we dropped all terms that go beyond our order of approximation.

4.3.2. Canonical quantisation and PZW transformation to a multipolar Hamiltonian

Now, we canonically quantise this Hamiltonian and perform the PZW transformation and electric dipole approximation used in [SB18] to arrive at the 'multipolar' Hamiltonian from ([SB18].23⋆). Neglecting terms of the form $\frac{\boldsymbol{p}_i\cdot[\boldsymbol{d}\times\boldsymbol{B}(\boldsymbol{R})]}{m_im_jc^2}$ as in ([SB18].22), in our gravitational correction terms from (4.3.3) these transformations amount just to the replacement $\bar{\boldsymbol{p}}_i \to \boldsymbol{p}_i$ (compare section (4.2.1) from ([SB18].14⋆) to ([SB18].21⋆)). Hence the multipolar Hamiltonian including the gravitational correction terms is

$$\begin{aligned} H_{[\mathrm{mult}],\mathrm{new}} = H_{[\mathrm{mult}]} &+ m_1\phi(\boldsymbol{r}_1) + m_2\phi(\boldsymbol{r}_2) + \frac{2\gamma+1}{2m_1c^2}\boldsymbol{p}_1\cdot\phi(\boldsymbol{r}_1)\boldsymbol{p}_1 + \frac{2\gamma+1}{2m_2c^2}\boldsymbol{p}_2\cdot\phi(\boldsymbol{r}_2)\boldsymbol{p}_2 \\ &+ (2\beta-1)\frac{m_1\phi(\boldsymbol{r}_1)^2}{2c^2} + (2\beta-1)\frac{m_2\phi(\boldsymbol{r}_2)^2}{2c^2}, \end{aligned} \tag{4.3.4}$$

where $H_{[\mathrm{mult}]}$ is the multipolar Hamiltonian from ([SB18].23⋆).

Now that we are on the quantum level, we had to choose a symmetrised operator ordering for the $\boldsymbol{p}^2\phi$ terms. We chose an ordering of the 'obvious' form $\boldsymbol{p}\cdot\phi\boldsymbol{p}$. As we have seen in section 3.4.3, this operator ordering also results from the description of single quantum particles in an Eddington–Robertson PPN metric by our WKB-like expansion of the Klein–Gordon equation, if we neglect terms proportional to $\Delta\phi$ (which vanish outside the matter generating the Newtonian potential ϕ, and thus are irrelevant in physical situations concerning the outside of the generating matter distribution).

4.3.3. Introduction of centre of mass variables

We now want to express the correction terms in (Newtonian) centre of mass and relative variables,

$$\boldsymbol{R} = \frac{m_1\boldsymbol{r}_1 + m_2\boldsymbol{r}_2}{M}\,, \qquad \boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2\,, \tag{4.3.5}$$

$$\boldsymbol{P} = \boldsymbol{p}_1 + \boldsymbol{p}_2\,, \qquad \boldsymbol{p}_{1,2} = \frac{m_{1,2}}{M}\boldsymbol{P} \pm \boldsymbol{p}_r\,, \tag{4.3.6}$$

where $M = m_1 + m_2$. To this end, we expand the gravitational potential ϕ around the centre of mass position $\boldsymbol{R}$ *in linear order*. In this approximation, we have $m_1\phi(\boldsymbol{r}_1) + m_2\phi(\boldsymbol{r}_2) = M\phi(\boldsymbol{R})$ and $m_1\phi(\boldsymbol{r}_1)^2 + m_2\phi(\boldsymbol{r}_2)^2 = M\phi(\boldsymbol{R})^2$. Furthermore using

$$\begin{aligned} \boldsymbol{p}_{1,2} \cdot \phi(\boldsymbol{r}_{1,2})\boldsymbol{p}_{1,2} &= \left(\frac{m_{1,2}}{M}\boldsymbol{P} \pm \boldsymbol{p}_{\boldsymbol{r}}\right) \cdot \phi(\boldsymbol{r}_{1,2}) \left(\frac{m_{1,2}}{M}\boldsymbol{P} \pm \boldsymbol{p}_{\boldsymbol{r}}\right) \\ &= \frac{m_{1,2}^2}{M^2}\boldsymbol{P} \cdot \phi(\boldsymbol{r}_{1,2})\boldsymbol{P} \pm \frac{m_{1,2}}{M}(\boldsymbol{P} \cdot \phi(\boldsymbol{r}_{1,2})\boldsymbol{p}_{\boldsymbol{r}} + \text{H.c.}) + \boldsymbol{p}_{\boldsymbol{r}} \cdot \phi(\boldsymbol{r}_{1,2})\boldsymbol{p}_{\boldsymbol{r}} \end{aligned} \tag{4.3.7}$$

and the relations $\phi(\boldsymbol{r}_1) - \phi(\boldsymbol{r}_2) = \boldsymbol{r} \cdot \boldsymbol{\nabla}\phi(\boldsymbol{R})$ as well as

$$\begin{aligned} \frac{1}{m_1}\phi(\boldsymbol{r}_1) + \frac{1}{m_2}\phi(\boldsymbol{r}_2) &= \left(\frac{1}{m_1} + \frac{1}{m_2}\right)\phi(\boldsymbol{R}) + \frac{1}{M}\left(\frac{m_2}{m_1} - \frac{m_1}{m_2}\right)\boldsymbol{r} \cdot \boldsymbol{\nabla}\phi(\boldsymbol{R}) \\ &= \frac{1}{\mu}\phi(\boldsymbol{R}) - \frac{m_1 - m_2}{m_1 m_2}\boldsymbol{r} \cdot \boldsymbol{\nabla}\phi(\boldsymbol{R}) \end{aligned} \tag{4.3.8}$$

where $\mu = \frac{m_1 m_2}{M}$ is the system's reduced mass, we arrive at the centre of mass Hamiltonian

$$\begin{aligned} H_{[\text{com}],\text{new}} = H_{[\text{com}]} &+ M\phi(\boldsymbol{R}) + (2\beta - 1)\frac{M\phi(\boldsymbol{R})^2}{2c^2} + \frac{2\gamma + 1}{2Mc^2}\boldsymbol{P} \cdot \phi(\boldsymbol{R})\boldsymbol{P} \\ &+ \frac{2\gamma + 1}{2\mu c^2}\boldsymbol{p}_{\boldsymbol{r}}^2\phi(\boldsymbol{R}) + \frac{2\gamma + 1}{2Mc^2}\left[\boldsymbol{P} \cdot (\boldsymbol{r} \cdot \boldsymbol{\nabla}\phi(\boldsymbol{R}))\boldsymbol{p}_{\boldsymbol{r}} + \text{H.c.}\right] \\ &- \frac{2\gamma + 1}{2c^2}\frac{m_1 - m_2}{m_1 m_2}\boldsymbol{p}_{\boldsymbol{r}} \cdot (\boldsymbol{r} \cdot \boldsymbol{\nabla}\phi(\boldsymbol{R}))\boldsymbol{p}_{\boldsymbol{r}}\,, \end{aligned} \tag{4.3.9}$$

where $H_{[\text{com}]}$ is the centre of mass Hamiltonian from ([SB18].25⋆).

This can, similarly to [SB18], be brought into the form

$$H_{[\text{com}],\text{new}} = H_{\text{C,new}} + H_{\text{A,new}} + H_{\text{AL}} + H_{\text{L}} + H_{\text{X}} + H_{\text{deriv,new}}, \tag{4.3.10}$$

where

$$H_{\text{C,new}} = H_{\text{C}} + \frac{2\gamma + 1}{2Mc^2}\boldsymbol{P} \cdot \phi(\boldsymbol{R})\boldsymbol{P} + \left(M + \frac{\boldsymbol{p}_{\boldsymbol{r}}^2}{2\mu c^2}\right)\phi(\boldsymbol{R}) + (2\beta - 1)\frac{M\phi(\boldsymbol{R})^2}{2c^2} \tag{4.3.11}$$

describes the dynamics of the centre of mass and

$$H_{\text{A,new}} = H_{\text{A}} + 2\gamma\frac{\phi(\boldsymbol{R})}{c^2}\frac{\boldsymbol{p}_{\boldsymbol{r}}^2}{2\mu} - \frac{2\gamma + 1}{2c^2}\frac{m_1 - m_2}{m_1 m_2}\boldsymbol{p}_{\boldsymbol{r}} \cdot (\boldsymbol{r} \cdot \boldsymbol{\nabla}\phi(\boldsymbol{R}))\boldsymbol{p}_{\boldsymbol{r}} \tag{4.3.12}$$

describes the internal dynamics of the atom, both modified in comparison to [SB18]. Here, we have included the term $2\gamma\frac{\phi(\boldsymbol{R})}{c^2}\frac{\boldsymbol{p}_{\boldsymbol{r}}^2}{2\mu}$ into $H_{\text{A,new}}$ since it can be combined with $\frac{\boldsymbol{p}_{\boldsymbol{r}}^2}{2\mu}$ from H_{A} into

$$\frac{\boldsymbol{p}_{\boldsymbol{r}}^2}{2\mu}\left(1 + 2\gamma\frac{\phi(\boldsymbol{R})}{c^2}\right) = \frac{{}^{(3)}g_R^{-1}(\boldsymbol{p}_{\boldsymbol{r}}, \boldsymbol{p}_{\boldsymbol{r}})}{2\mu}, \tag{4.3.13}$$

giving the geometrically correctly expressed Newtonian internal kinetic energy, using the metric square of the internal momentum. Here ${}^{(3)}g_{\boldsymbol{R}}^{-1}$ denotes the inverse of the physical spatial metric at position $\boldsymbol{R}$, as explained in section 2.2.

The terms H_{AL}, H_{L}, and H_{X} containing, respectively, the atom-light interaction terms, the external electromagnetic field energy, and the 'cross terms' are not changed compared to [SB18]. The new final summand

$$H_{\mathrm{deriv,new}} = \frac{2\gamma+1}{2Mc^2}[\boldsymbol{P}\cdot(\boldsymbol{r}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{R}))\boldsymbol{p}_{\boldsymbol{r}} + \mathrm{H.c.}] \tag{4.3.14}$$

is an additional central–internal 'cross term' involving the derivative $\boldsymbol{\nabla}\phi$ of the gravitational potential.

Note that if we assumed that the gravitational potential ϕ vary slowly over the extension of the atom, we could neglect the terms $\boldsymbol{r}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{R})$. However, such terms might turn out interesting for experimental applications employing large superpositions.

4.4. Coupling the gravitational to the electromagnetic field

Having determined the gravitational field's coupling to the particles in the previous section, we now turn to its coupling to the electromagnetic field, whose Lagrangian in the presence of gravity we will compute in this section. In the following section 4.5 we will then combine all couplings into a single Hamiltonian.

4.4.1. Solution of the gravitationally modified Maxwell equations

The electromagnetic part of the total action of our system, including interaction with matter, is

$$S_{\mathrm{em}} = \int \mathrm{d}t\,\mathrm{d}^3\boldsymbol{x}\,\sqrt{-g}\left(-\frac{\varepsilon_0 c^2}{4}F_{\mathrm{tot.}\mu\nu}F_{\mathrm{tot.}}^{\mu\nu} + J^\mu A_{\mathrm{tot.}\mu}\right), \tag{4.4.1}$$

where g denotes the determinant of the matrix $(g_{\mu\nu})$ of metric components, $J = J^\mu\partial_\mu$ is the four-current 'density' vector field, $A_{\mathrm{tot.}} = A_{\mathrm{tot.}\mu}\mathrm{d}x^\mu$ is the total (i.e. not decomposed into internal and external parts) electromagnetic four-potential form, and $\mathrm{d}A_{\mathrm{tot.}} = F_{\mathrm{tot.}} = F_{\mathrm{tot.}\mu\nu}\mathrm{d}x^\mu\otimes\mathrm{d}x^\nu = (\partial_\mu A_{\mathrm{tot.}\nu} - \partial_\nu A_{\mathrm{tot.}\mu})\mathrm{d}x^\mu\otimes\mathrm{d}x^\nu$ is the electromagnetic field tensor. This is the standard action describing electromagnetism in a gravitational field, which is obtained by minimally coupling the special-relativistic action for electromagnetism [Jac98] to a general spacetime metric [MTW73; HE73].

Note that J^μ are the components of a proper vector field and not of a density; their relation to the four-current *density* with components j^μ, in terms of which the interaction part of the action takes the form $\int \mathrm{d}t\, \mathrm{d}^3\boldsymbol{x}\, j^\mu A_{\mathrm{tot.}\mu}$, is given by

$$J^\mu = \frac{1}{\sqrt{-g}} j^\mu. \tag{4.4.2}$$

The current density of our system of two particles is given by[7]

$$j^\mu(t, \boldsymbol{x}) = \sum_{i=1}^{2} e_i \delta^{(3)}(\boldsymbol{x} - \boldsymbol{r}_i(t)) \dot{r}_i^\mu(t), \tag{4.4.3}$$

where the dot denotes differentiation with respect to coordinate time t. The charge density is

$$\rho = \frac{1}{c} j^0. \tag{4.4.4}$$

Similarly, the electric potential is

$$\phi_{\mathrm{el.,tot.}} = -c A_{\mathrm{tot.}0}. \tag{4.4.5}$$

The Maxwell equations obtained by varying the action with respect to $A_{\mathrm{tot.}\mu}$ take the form

$$\nabla_\mu F^{\mu\nu}_{\mathrm{tot.}} = -\frac{1}{\varepsilon_0 c^2} J^\nu \tag{4.4.6}$$

in terms of the current vector field, or

$$\nabla_\mu F^{\mu\nu}_{\mathrm{tot.}} = -\frac{1}{\varepsilon_0 c^2} \frac{1}{\sqrt{-g}} j^\nu \tag{4.4.7}$$

in terms of the current density. It will be useful to consider the form

$$\nabla^\mu F_{\mathrm{tot.}\mu\nu} = -\frac{1}{\varepsilon_0 c^2} \frac{1}{\sqrt{-g}} j_\nu \tag{4.4.8}$$

instead.

We employ the 'background Coulomb gauge' condition

$$0 = \boldsymbol{\nabla} \cdot \boldsymbol{A}_{\mathrm{tot.}} = \delta^{ab} \partial_a A_{\mathrm{tot.}b}, \tag{4.4.9}$$

implying in particular $\delta^{ab}\partial_a F_{\mathrm{tot.}b\mu} = \Delta A_{\mathrm{tot.}\mu}$ where $\Delta = \delta^{ab}\partial_a\partial_b$ denotes the 'flat' Euclidean Laplacian defined by the background structures. In terms of the Helmholtz decomposition, the gauge condition means $\boldsymbol{A}^{\parallel}_{\mathrm{tot.}} = 0$, i.e. $\boldsymbol{A}_{\mathrm{tot.}} = \boldsymbol{A}^{\perp}_{\mathrm{tot.}}$.

[7] For a single particle of charge q on an arbitrarily parametrised timelike worldline $r^\mu(\lambda)$, the current density is given by

$$j^\mu(x) = qc \int \mathrm{d}\lambda\, \frac{\mathrm{d}r^\mu}{\mathrm{d}\lambda} \delta^{(4)}(x - r(\lambda)).$$

Parametrising by coordinate time and considering two particles, we arrive at the above expression.

Divergence of the field strength tensor

Using the Christoffel symbols of the Eddington–Robertson PPN metric, which are computed in full detail in appendix B, we can now calculate the components of the divergence of the field strength tensor $F_{\text{tot.}}$. For the calculations, we remind the reader that the components of the field tensor are of the orders $F_{\text{tot.}a0} = \mathrm{O}(c^{-1})$ and $F_{\text{tot.}ab} = \mathrm{O}(c^0)$, as explained in section 2.4. The 0 component of the divergence now is as follows:

$$\begin{aligned}
\nabla^\mu F_{\text{tot.}\mu 0} &= g^{\mu\rho}(\partial_\rho F_{\text{tot.}\mu 0} - \Gamma^\sigma_{\rho\mu} F_{\text{tot.}\sigma 0} - \Gamma^\sigma_{\rho 0} F_{\text{tot.}\mu\sigma}) \\
&= \underbrace{g^{a\rho}\partial_\rho F_{\text{tot.}a0}}_{=g^{ab}\partial_b F_{\text{tot.}a0}+\mathrm{O}(c^{-7})} - g^{\mu\rho}\Gamma^a_{\rho\mu} F_{\text{tot.}a0} - \underbrace{g^{\mu\rho}\Gamma^\sigma_{\rho 0} F_{\text{tot.}\mu\sigma}}_{=g^{00}\Gamma^a_{00}F_{\text{tot.}0a}+g^{ab}\Gamma^0_{b0}F_{\text{tot.}a0}+g^{ab}\Gamma^c_{b0}F_{\text{tot.}ac}+\mathrm{O}(c^{-7})} \\
&= \left(1 + 2\gamma\frac{\phi}{c^2}\right)\delta^{ab}\partial_b F_{\text{tot.}a0} - (\gamma - 1)\delta^{ab}\frac{\partial_b\phi}{c^2} F_{\text{tot.}a0} + \delta^{ab}\frac{\partial_b\phi}{c^2} F_{\text{tot.}0a} - \delta^{ab}\frac{\partial_b\phi}{c^2} F_{\text{tot.}a0} \\
&\quad + \cancelto{0}{\delta^{ab}\gamma\delta^c_b\frac{\partial_t\phi}{c^3} F_{\text{tot.}ac}} + \mathrm{O}(c^{-5}) \\
&= \left(1 + 2\gamma\frac{\phi}{c^2}\right)\Delta A_{\text{tot.}0} - (\gamma + 1)\delta^{ab}\frac{\partial_b\phi}{c^2}(\partial_a A_{\text{tot.}0} - \partial_0 A^\perp_{\text{tot.}a}) + \mathrm{O}(c^{-5}) \\
&= -\frac{1}{c}\left(1 + 2\gamma\frac{\phi}{c^2}\right)\Delta\phi_{\text{el.,tot.}} + (\gamma + 1)\delta^{ab}\frac{\partial_b\phi}{c^3}(\partial_a\phi_{\text{el.,tot.}} + \partial_t A^\perp_{\text{tot.}a}) + \mathrm{O}(c^{-5})
\end{aligned} \tag{4.4.10}$$

Employing 'three-vector' notation as introduced in section 2.3, this is equivalent to

$$c\nabla^\mu F_{\text{tot.}\mu 0} = -\left(1 + 2\gamma\frac{\phi}{c^2}\right)\Delta\phi_{\text{el.,tot.}} + (\gamma + 1)\frac{\boldsymbol{\nabla}\phi}{c^2}\cdot(\boldsymbol{\nabla}\phi_{\text{el.,tot.}} + \partial_t \boldsymbol{A}^\perp_{\text{tot.}}) + \mathrm{O}(c^{-4}), \tag{4.4.11}$$

or (multiplying by $(1 - 2\gamma\frac{\phi}{c^2})$) to

$$\Delta\phi_{\text{el.,tot.}} = -\left(1 - 2\gamma\frac{\phi}{c^2}\right)c\nabla^\mu F_{\text{tot.}\mu 0} + (\gamma + 1)\frac{\boldsymbol{\nabla}\phi}{c^2}\cdot(\boldsymbol{\nabla}\phi_{\text{el.,tot.}} + \partial_t \boldsymbol{A}^\perp_{\text{tot.}}) + \mathrm{O}(c^{-4}). \tag{4.4.12}$$

For the spatial components, we obtain

$$\begin{aligned}
\nabla^\mu F_{\text{tot.}\mu a} &= g^{\mu\rho}(\partial_\rho F_{\text{tot.}\mu a} - \Gamma^\sigma_{\rho\mu} F_{\text{tot.}\sigma a} - \Gamma^\sigma_{\rho a} F_{\text{tot.}\mu\sigma}) \\
&= g^{00}\partial_0 F_{\text{tot.}0a} + g^{bc}\partial_c F_{ba} - \underbrace{g^{\mu\rho}\Gamma^0_{\rho\mu}}_{=\mathrm{O}(c^{-3})} F_{\text{tot.}0a} - \underbrace{g^{\mu\rho}\Gamma^b_{\rho\mu}}_{=(\gamma-1)\delta^{bc}\frac{\partial_c\phi}{c^2}+\mathrm{O}(c^{-4})} F_{\text{tot.}ba} \\
&\quad - \underbrace{g^{\mu\rho}\Gamma^\sigma_{\rho a} F_{\text{tot.}\mu\sigma}}_{=g^{00}\Gamma^b_{0a}F_{\text{tot.}0b}+g^{bc}\Gamma^\sigma_{ca}F_{\text{tot.}b\sigma}+\mathrm{O}(c^{-7})} + \mathrm{O}(c^{-6})
\end{aligned}$$

$$
\begin{aligned}
&= -\partial_0 F_{\text{tot}.0a} + \left(1 + 2\gamma\frac{\phi}{c^2}\right)\delta^{bc}\partial_c F_{\text{tot}.ba} - (\gamma-1)\delta^{bc}\frac{\partial_c\phi}{c^2}F_{\text{tot}.ba} \\
&\quad - \underbrace{\delta^{bc}\Gamma^d_{ca}F_{\text{tot}.bd}}_{=-2\gamma\delta^{bc}\frac{\partial_c\phi}{c^2}F_{\text{tot}.ba}+\mathrm{O}(c^{-4})} + \mathrm{O}(c^{-4}) \\
&= -\frac{1}{c^2}\partial_t(\partial_t A^{\perp}_{\text{tot}.a} + \partial_a\phi_{\text{el.,tot.}}) + \left(1 + 2\gamma\frac{\phi}{c^2}\right)\Delta A^{\perp}_{\text{tot}.a} \\
&\quad + (\gamma+1)\delta^{bc}\frac{\partial_c\phi}{c^2}(\partial_b A^{\perp}_{\text{tot}.a} - \partial_a A^{\perp}_{\text{tot}.b}) + \mathrm{O}(c^{-4}).
\end{aligned}
\tag{4.4.13}
$$

Multiplying by $(1 - 2\gamma\frac{\phi}{c^2})$, this is equivalent to

$$
\begin{aligned}
(\Delta - c^{-2}\partial_t^2)A^{\perp}_{\text{tot}.a} &= \left(1 - 2\gamma\frac{\phi}{c^2}\right)\nabla^{\mu}F_{\text{tot}.\mu a} + \frac{1}{c^2}\partial_a\partial_t\phi_{\text{el.,tot.}} \\
&\quad - (\gamma+1)\delta^{bc}\frac{\partial_c\phi}{c^2}(\partial_b A^{\perp}_{\text{tot}.a} - \partial_a A^{\perp}_{\text{tot}.b}) + \mathrm{O}(c^{-4}).
\end{aligned}
\tag{4.4.14}
$$

The source terms and the explicit form of the Maxwell equations

We now consider the right hand side of the Maxwell equations (4.4.8), i.e. the source term $-\frac{1}{\varepsilon_0 c^2}\frac{1}{\sqrt{-g}}j_\nu$. Using

$$
\frac{1}{\sqrt{-g}} = 1 + (3\gamma - 1)\frac{\phi}{c^2} + \mathrm{O}(c^{-4})
\tag{4.4.15}
$$

and the metric coefficients, we can easily express the source term in terms of the charge and current densities: the 0 component is

$$
\begin{aligned}
-\frac{1}{\varepsilon_0 c^2}\frac{1}{\sqrt{-g}}j_0 &= -\frac{1}{\varepsilon_0 c^2}\frac{1}{\sqrt{-g}}(g_{00}j^0 + \underbrace{g_{0a}j^a}_{=\mathrm{O}(c^{-5})}) \\
&= \frac{1}{\varepsilon_0 c}\frac{1}{\sqrt{-g}}(-g_{00}\rho + \mathrm{O}(c^{-6})) \\
&= \frac{1}{\varepsilon_0 c}\left(1 + (3\gamma+1)\frac{\phi}{c^2}\right)\rho + \mathrm{O}(c^{-5}),
\end{aligned}
\tag{4.4.16}
$$

and the spatial components are

$$
\begin{aligned}
-\frac{1}{\varepsilon_0 c^2}\frac{1}{\sqrt{-g}}j_a &= -\frac{1}{\varepsilon_0 c^2}\frac{1}{\sqrt{-g}}(g_{ab}j^b + \underbrace{g_{a0}j^0}_{=\mathrm{O}(c^{-4})}) \\
&= -\frac{1}{\varepsilon_0 c^2}\left(1 + (\gamma-1)\frac{\phi}{c^2}\right)\delta_{ab}j^b + \mathrm{O}(c^{-6}).
\end{aligned}
\tag{4.4.17}
$$

Using the source terms (4.4.16), (4.4.17) and the re-arranged field strength divergences (4.4.12), (4.4.14), the Maxwell equations (4.4.8) are equivalent to the following equations:

$$\begin{aligned}\Delta\phi_{\text{el.,tot.}} &= -\frac{1}{\varepsilon_0}\left(1+(\gamma+1)\frac{\phi}{c^2}\right)\rho \\ &\quad + (\gamma+1)\frac{\boldsymbol{\nabla}\phi}{c^2}\cdot(\boldsymbol{\nabla}\phi_{\text{el.,tot.}}+\partial_t \boldsymbol{A}^{\perp}_{\text{tot.}}) + \mathrm{O}(c^{-4}) \qquad (4.4.18a)\\ (\Delta - c^{-2}\partial_t^2)A^{\perp}_{\text{tot.}a} &= -\frac{1}{\varepsilon_0 c^2}\delta_{ab}j^b + \frac{1}{c^2}\partial_a\partial_t\phi_{\text{el.,tot.}} \\ &\quad - (\gamma+1)\delta^{bc}\frac{\partial_c\phi}{c^2}(\partial_b A^{\perp}_{\text{tot.}a} - \partial_a A^{\perp}_{\text{tot.}b}) + \mathrm{O}(c^{-4}) \qquad (4.4.18b)\end{aligned}$$

Now, as done in [SB18], we split the total potentials $(\phi_{\text{el.,tot.}}, \boldsymbol{A}^{\perp}_{\text{tot.}})$ into internal and external parts, both satisfying the gauge condition, where the internal potentials $(\phi_{\text{el.}}, \boldsymbol{\mathcal{A}}^{\perp})$ satisfy the Maxwell equations with the internal charge and current densities as sources, and the external potentials $(\phi_{\text{el.,ext.}}, \boldsymbol{A}^{\perp})$ the vacuum Maxwell equations. Note that the internal electric potential does not carry a subscript 'int.' or similar, as opposed to the external one. Similarly, we write $F_{\text{tot.}\mu\nu} = \mathcal{F}_{\mu\nu} + F_{\mu\nu}$, where $\mathcal{F} = \mathrm{d}\mathcal{A}$ is the internal and $F = \mathrm{d}A$ is the external field tensor (employing the obvious notation $\mathcal{A}_0 = -\frac{1}{c}\phi_{\text{el.}}$, $A_0 = -\frac{1}{c}\phi_{\text{el.,ext.}}$).

Solution of the internal Maxwell equations

From (4.4.18), the Maxwell equations for the internal potentials are as follows:

$$\Delta\phi_{\text{el.}} = -\frac{1}{\varepsilon_0}\left(1+(\gamma+1)\frac{\phi}{c^2}\right)\rho + (\gamma+1)\frac{\boldsymbol{\nabla}\phi}{c^2}\cdot(\boldsymbol{\nabla}\phi_{\text{el.}}+\partial_t\boldsymbol{\mathcal{A}}^{\perp}) + \mathrm{O}(c^{-4}) \qquad (4.4.19a)$$

$$\begin{aligned}(\Delta - c^{-2}\partial_t^2)\mathcal{A}^{\perp}_a &= -\frac{1}{\varepsilon_0 c^2}\delta_{ab}j^b + \frac{1}{c^2}\partial_a\partial_t\phi_{\text{el.}} \\ &\quad - (\gamma+1)\delta^{bc}\frac{\partial_c\phi}{c^2}(\partial_b\mathcal{A}^{\perp}_a - \partial_a\mathcal{A}^{\perp}_b) + \mathrm{O}(c^{-4}) \qquad (4.4.19b)\end{aligned}$$

We will now solve (4.4.19) perturbatively in a formal expansion in c^{-2}. Expanding the potentials as $\phi_{\text{el.}} = \phi^{(0)}_{\text{el.}} + c^{-2}\phi^{(2)}_{\text{el.}} + \mathrm{O}(c^{-4})$ and $\boldsymbol{\mathcal{A}}^{\perp} = \boldsymbol{\mathcal{A}}^{\perp(0)} + c^{-2}\boldsymbol{\mathcal{A}}^{\perp(2)} + \mathrm{O}(c^{-4})$, the lowest orders of the Poisson equation for $\phi_{\text{el.}}$ read

$$\Delta\phi^{(0)}_{\text{el.}} = -\frac{1}{\varepsilon_0}\rho, \qquad (4.4.20a)$$

$$\Delta\phi^{(2)}_{\text{el.}} = -\frac{1}{\varepsilon_0}(\gamma+1)\phi\rho + (\gamma+1)\boldsymbol{\nabla}\phi\cdot(\boldsymbol{\nabla}\phi^{(0)}_{\text{el.}} + \partial_t\boldsymbol{\mathcal{A}}^{\perp(0)}), \qquad (4.4.20b)$$

and the lowest orders of the wave equation for $\boldsymbol{\mathcal{A}}^{\perp}$ are

$$(\Delta - c^{-2}\partial_t^2)\mathcal{A}_a^{\perp(0)} = 0, \tag{4.4.21a}$$

$$(\Delta - c^{-2}\partial_t^2)\mathcal{A}_a^{\perp(2)} = -\frac{1}{\varepsilon_0}\delta_{ab}j^b + \partial_a\partial_t\phi_{\text{el.}}^{(0)} - (\gamma+1)\delta^{bc}\frac{\partial_c\phi}{c^2}(\partial_b\mathcal{A}_a^{\perp(0)} - \partial_a\mathcal{A}_b^{\perp(0)}). \tag{4.4.21b}$$

Being the usual, 'non-gravitational' Poisson equation, (4.4.20a) gives

$$\phi_{\text{el.}}^{(0)} = \phi_{\text{el.,ng}}\,, \tag{4.4.22}$$

where $\phi_{\text{el.,ng}}$ is the internal electric potential solution in the absence of gravity as given by ([SB18].A1).

For the wave equation (4.4.19b) we are interested in purely retarded solutions without any additional radiative terms, since the internal potentials shall correspond to just 'what is generated by the particles'. Therefore, (4.4.21a) directly implies $\boldsymbol{\mathcal{A}}^{\perp(0)} = 0$.

Thus, (4.4.21b) reduces to the 'non-gravitational' wave equation for the potential $\boldsymbol{\mathcal{A}}_{\text{ng}}^{\perp}$, but applied to $c^{-2}\boldsymbol{\mathcal{A}}^{\perp(2)}$, implying $c^{-2}\boldsymbol{\mathcal{A}}^{\perp(2)} = \boldsymbol{\mathcal{A}}_{\text{ng}}^{\perp}$, where $\boldsymbol{\mathcal{A}}_{\text{ng}}^{\perp}$ is the non-gravitational retarded solution, expanded to lowest non-vanishing order in c^{-1}, as given by ([SB18].A3). Hence we have

$$\boldsymbol{\mathcal{A}}^{\perp} = \boldsymbol{\mathcal{A}}_{\text{ng}}^{\perp} + \mathrm{O}(c^{-4}) = \mathrm{O}(c^{-2}). \tag{4.4.23}$$

Finally, solving (4.4.20b) directly gives

$$\phi_{\text{el.}}^{(2)}(\boldsymbol{x},t) = \frac{\gamma+1}{4\pi\varepsilon_0}\int \mathrm{d}^3x'\,\frac{\phi(\boldsymbol{x}',t)\rho(\boldsymbol{x}',t)}{|\boldsymbol{x}-\boldsymbol{x}'|} - \frac{\gamma+1}{4\pi}\int \mathrm{d}^3x'\,\frac{1}{|\boldsymbol{x}-\boldsymbol{x}'|}\left(\boldsymbol{\nabla}\phi\cdot\boldsymbol{\nabla}\phi_{\text{el.}}^{(0)}\right)(\boldsymbol{x}',t). \tag{4.4.24}$$

For later convenience, we will now compute the interaction integral $-\frac{1}{2}\int \mathrm{d}^3\boldsymbol{x}\,\rho\phi_{\text{el.}}$. We suppress time dependence in the notation. Using the explicit form of the charge density, $\rho(\boldsymbol{x}) = e_1\delta^{(3)}(\boldsymbol{x}-\boldsymbol{r}_1) + e_2\delta^{(3)}(\boldsymbol{x}-\boldsymbol{r}_2)$, and dropping infinite self-interaction terms, we obtain

$$\begin{aligned}-\frac{1}{2}\int \mathrm{d}^3\boldsymbol{x}\,\rho\phi_{\text{el.}} = &-\frac{e_1e_2}{4\pi\varepsilon_0 r}\left(1 + (\gamma+1)\frac{\phi(\boldsymbol{r}_1)+\phi(\boldsymbol{r}_2)}{2c^2}\right)\\ &+ \underbrace{\frac{\gamma+1}{8\pi c^2}\int \mathrm{d}^3\boldsymbol{x}\left(\frac{e_1}{|\boldsymbol{x}-\boldsymbol{r}_1|}+\frac{e_2}{|\boldsymbol{x}-\boldsymbol{r}_2|}\right)\boldsymbol{\nabla}\phi\cdot\boldsymbol{\nabla}\phi_{\text{el.}}^{(0)}}_{=\frac{\varepsilon_0(\gamma+1)}{2c^2}\int \mathrm{d}^3\boldsymbol{x}\,\phi_{\text{el.}}^{(0)}\boldsymbol{\nabla}\phi\cdot\boldsymbol{\nabla}\phi_{\text{el.}}^{(0)}} + \mathrm{O}(c^{-4}),\end{aligned} \tag{4.4.25}$$

where we used the explicit form of the lowest-order potential $\phi_{\text{el.}}^{(0)}$. For the last integral, partial integration gives

$$\begin{aligned}\int \mathrm{d}^3\boldsymbol{x}\, \phi_{\text{el.}}^{(0)} \boldsymbol{\nabla}\phi \cdot \boldsymbol{\nabla}\phi_{\text{el.}}^{(0)} &= -\int \mathrm{d}^3\boldsymbol{x}\, \phi_{\text{el.}}^{(0)} \boldsymbol{\nabla} \cdot \left(\phi_{\text{el.}}^{(0)} \boldsymbol{\nabla}\phi\right) \\ &= -\int \mathrm{d}^3\boldsymbol{x}\, \phi_{\text{el.}}^{(0)} \boldsymbol{\nabla}\phi_{\text{el.}}^{(0)} \cdot \boldsymbol{\nabla}\phi - \int \mathrm{d}^3\boldsymbol{x} \left(\phi_{\text{el.}}^{(0)}\right)^2 \Delta\phi, \end{aligned} \tag{4.4.26}$$

implying

$$\int \mathrm{d}^3\boldsymbol{x}\, \phi_{\text{el.}}^{(0)} \boldsymbol{\nabla}\phi \cdot \boldsymbol{\nabla}\phi_{\text{el.}}^{(0)} = -\frac{1}{2} \int \mathrm{d}^3\boldsymbol{x} \left(\phi_{\text{el.}}^{(0)}\right)^2 \Delta\phi. \tag{4.4.27}$$

In the following, we will neglect this term: due to the Newtonian field equation, $\Delta\phi$ is non-vanishing only inside the matter generating the gravitational potential, and $\phi_{\text{el.}}^{(0)}$ is negligibly small there for an atom situated outside of this matter (e.g. in a quantum-optical experiment outside of the earth). Thus, the relevant part of the above interaction integral is just

$$-\frac{1}{2} \int \mathrm{d}^3\boldsymbol{x}\, \rho \phi_{\text{el.}} = -\frac{e_1 e_2}{4\pi\varepsilon_0 r} \left(1 + (\gamma+1) \frac{\phi(\boldsymbol{r}_1) + \phi(\boldsymbol{r}_2)}{2c^2}\right) + \mathrm{O}(c^{-4}). \tag{4.4.28}$$

The external Maxwell equations

We will now consider the Maxwell equations for the external potentials. Since we assume the absence of external charges, the Poisson equation for $\phi_{\text{el.,ext.}}$ reads as follows:

$$\Delta\phi_{\text{el.,ext.}} = (\gamma+1) \frac{\boldsymbol{\nabla}\phi}{c^2} \cdot (\boldsymbol{\nabla}\phi_{\text{el.,ext.}} + \partial_t \boldsymbol{A}^{\perp}) + \mathrm{O}(c^{-4}) \tag{4.4.29}$$

Solving this equation perturbatively as for the internal potentials, we obtain the solution

$$\phi_{\text{el.,ext.}}(\boldsymbol{x}, t) = -\frac{\gamma+1}{4\pi c^2} \int \mathrm{d}^3\boldsymbol{x}' \frac{1}{|\boldsymbol{x} - \boldsymbol{x}'|} (\boldsymbol{\nabla}\phi \cdot \partial_t \boldsymbol{A}^{\perp})(\boldsymbol{x}', t) + \mathrm{O}(c^{-4}), \tag{4.4.30}$$

expressed solely in terms of the external vector potential. In fact, we will not need this explicit form of the potential, but just the expansion order

$$\phi_{\text{el.,ext.}} = \mathrm{O}(c^{-2}). \tag{4.4.31}$$

Now considering the wave equation for the vector potential $\boldsymbol{A}^{\perp}$, which due to the absence of external currents and the above result on $\phi_{\text{el.,ext.}}$ reads

$$\begin{aligned}(\Delta - c^{-2}\partial_t^2)A_a^{\perp} &= \frac{1}{c^2}\partial_a\partial_t\phi_{\text{el.,ext.}} - (\gamma+1)\delta^{bc}\frac{\partial_c\phi}{c^2}(\partial_b A_a^{\perp} - \partial_a A_b^{\perp}) + \mathrm{O}(c^{-4}) \\ &= -(\gamma+1)\delta^{bc}\frac{\partial_c\phi}{c^2}(\partial_b A_a^{\perp} - \partial_a A_b^{\perp}) + \mathrm{O}(c^{-4}),\end{aligned} \tag{4.4.32}$$

and employing a further expansion $\boldsymbol{A}^{\perp} = \boldsymbol{A}^{\perp(0)} + c^{-2}\boldsymbol{A}^{\perp(2)} + \mathrm{O}(c^{-4})$, we obtain in lowest order

$$(\Delta - c^{-2}\partial_t^2)\boldsymbol{A}^{\perp(0)} = 0. \tag{4.4.33}$$

Differently to the internal case, we now allow for radiative solutions[8], thus *not* getting $\boldsymbol{A}^{\perp(0)} = 0$. However, we can conclude that $\partial_a\boldsymbol{A}^{\perp} = \mathrm{O}(c^{-1}\partial_t\boldsymbol{A}^{\perp})$. Treating $\partial_t\boldsymbol{A}^{\perp}$, which corresponds (up to a gravitational correction factor of order unity) to the external electric field, as being of order c^0, we thus have

$$\partial_a\boldsymbol{A}^{\perp} = \mathrm{O}(c^{-1}). \tag{4.4.34}$$

4.4.2. Computation of the electromagnetic Lagrangian

We will now compute the electromagnetic Lagrangian

$$L_{\text{em}} = \int \mathrm{d}^3\boldsymbol{x}\,\left(-\frac{\varepsilon_0 c^2}{4}\sqrt{-g}\,F_{\text{tot.}\mu\nu}F_{\text{tot.}}^{\mu\nu} + j^{\mu}A_{\text{tot.}\mu}\right), \tag{4.4.35}$$

which follows from the action (4.4.1).

The internal kinetic Maxwell term is

$$\begin{aligned}&-\frac{\varepsilon_0 c^2}{4}\int \mathrm{d}^3\boldsymbol{x}\,\sqrt{-g}\,\mathcal{F}_{\mu\nu}\mathcal{F}^{\mu\nu} \\ &\quad= -\frac{\varepsilon_0 c^2}{2}\int \mathrm{d}^3\boldsymbol{x}\,\sqrt{-g}\,\partial_{\mu}\mathcal{A}_{\nu}\mathcal{F}^{\mu\nu} \\ (\text{P.I.})\quad &\quad= \frac{\varepsilon_0 c^2}{2}\int \mathrm{d}^3\boldsymbol{x}\,\sqrt{-g}\,\mathcal{A}_{\nu}\nabla_{\mu}\mathcal{F}^{\mu\nu} - \frac{\varepsilon_0 c^2}{2}\int \mathrm{d}^3\boldsymbol{x}\,\partial_0(\sqrt{-g}\mathcal{A}_{\nu}\mathcal{F}^{0\nu}).\end{aligned} \tag{4.4.36}$$

[8] At the end of the day, the idea is to put an atom into a laser beam.

The first integral on the right-hand side is equal to $-\frac{1}{2}\int \mathrm{d}^3\boldsymbol{x}\,\mathcal{A}_\nu j^\nu$ by the internal part of the general Maxwell equations (4.4.7), and for the second integral we obtain

$$\begin{aligned}
&-\frac{\varepsilon_0 c^2}{2}\int \mathrm{d}^3\boldsymbol{x}\,\partial_0(\sqrt{-g}\,\mathcal{A}_\nu\mathcal{F}^{0\nu}) \\
&\quad= -\frac{\varepsilon_0 c^2}{2}\int \mathrm{d}^3\boldsymbol{x}\,\partial_0(\sqrt{-g}\,\mathcal{A}_a\mathcal{F}^{0a}) \\
&\qquad\text{(using } \mathcal{F}^{0a} = g^{00}g^{ab}\mathcal{F}_{0b} + \mathrm{O}(c^{-5})) \\
&\quad= -\frac{\varepsilon_0 c^2}{2}\int \mathrm{d}^3\boldsymbol{x}\,\partial_0\left(\sqrt{-g}\,g^{00}g^{ab}\mathcal{A}_a(\partial_0\mathcal{A}_b - \partial_b\mathcal{A}_0)\right) + \mathrm{O}(c^{-4}) \\
&\quad= -\frac{\varepsilon_0}{2}\int \mathrm{d}^3\boldsymbol{x}\,\partial_t\left(\sqrt{-g}\,g^{00}g^{ab}\mathcal{A}_a(\partial_t\mathcal{A}_b + \partial_b\phi_{\text{el.}})\right) + \mathrm{O}(c^{-4}) \\
\text{(P.I.)}&\quad= -\frac{\varepsilon_0}{2}\int \mathrm{d}^3\boldsymbol{x}\,\partial_t\left(\sqrt{-g}\,g^{00}g^{ab}\mathcal{A}_a\partial_t\mathcal{A}_b\right) \\
&\qquad+ \frac{\varepsilon_0}{2}\int \mathrm{d}^3\boldsymbol{x}\,\partial_t\Big(\underbrace{\partial_b\left(\sqrt{-g}\,g^{00}g^{ab}\right)}_{=\mathrm{O}(c^{-2})}\mathcal{A}_a\phi_{\text{el.}}\Big) \\
&\qquad+ \frac{\varepsilon_0}{2}\int \mathrm{d}^3\boldsymbol{x}\,\partial_t\Big(\sqrt{-g}\,g^{00}\underbrace{g^{ab}\partial_b\mathcal{A}_a}_{=(1+2\gamma\frac{\phi}{c^2})\delta^{ab}\partial_b\mathcal{A}_a^\perp+\mathrm{O}(c^{-4})=\mathrm{O}(c^{-4})}\phi_{\text{el.}}\Big) + \mathrm{O}(c^{-4}) \\
&\quad= \mathrm{O}(c^{-4}),
\end{aligned} \tag{4.4.37}$$

where in the partial integration step we used the gauge condition (4.4.9) and that $\mathcal{A}_a$ is of order c^{-2} according to (4.4.23). Thus, the 'purely internal' contribution of electromagnetism to the Lagrangian, including the explicit coupling term of the internal potential to the current, is

$$\begin{aligned}
L_{\text{em,int.}} &= \int \mathrm{d}^3\boldsymbol{x}\left(-\frac{\varepsilon_0 c^2}{4}\sqrt{-g}\,\mathcal{F}_{\mu\nu}\mathcal{F}^{\mu\nu} + j^\mu\mathcal{A}_\mu\right) \\
&= \frac{1}{2}\int \mathrm{d}^3\boldsymbol{x}\,j^\mu\mathcal{A}_\mu + \mathrm{O}(c^{-4}) \\
&= \frac{1}{2}\int \mathrm{d}^3\boldsymbol{x}\,(\boldsymbol{j}\cdot\boldsymbol{\mathcal{A}}^\perp - \rho\phi_{\text{el.}}) + \mathrm{O}(c^{-4}).
\end{aligned} \tag{4.4.38}$$

To compute the purely external and mixed external-internal contributions to the electromagnetic Lagrangian, we first explicitly compute the kinetic Maxwell term in terms of the potentials. Inserting the explicit form of the PPN metric, we obtain

$$\begin{aligned}
-\frac{\varepsilon_0 c^2}{4}\sqrt{-g}\,F_{\text{tot.}\mu\nu}F_{\text{tot.}}^{\mu\nu} = \frac{\varepsilon_0}{2}\sqrt{-g}\,\Big[&-g^{00}g^{ab}(\partial_t A_{\text{tot.}a} + \partial_a\phi_{\text{el.,tot.}})(\partial_t A_{\text{tot.}b} + \partial_b\phi_{\text{el.,tot.}}) \\
&- c^2(g^{ab}g^{cd} - g^{ad}g^{cb})\,\partial_a A_{\text{tot.}c}\,\partial_b A_{\text{tot.}d}\Big] + \mathrm{O}(c^{-4})
\end{aligned}$$

$$
\begin{aligned}
&= \frac{\varepsilon_0}{2}\left[\left(1-(\gamma+1)\frac{\phi}{c^2}\right)(\partial_t \boldsymbol{A}_{\text{tot.}} + \boldsymbol{\nabla}\phi_{\text{el.,tot.}})^2\right.\\
&\qquad \left. - c^2\left(1+(\gamma+1)\frac{\phi}{c^2}\right)(\boldsymbol{\nabla}\times\boldsymbol{A}_{\text{tot.}})^2\right] + \mathrm{O}(c^{-4}). \qquad (4.4.39)
\end{aligned}
$$

Note that according to (4.4.23) and (4.4.34) we have $\boldsymbol{\nabla}\times\boldsymbol{A}_{\text{tot.}} = \mathrm{O}(c^{-1})$, such that the second term in the square brackets does indeed include terms up to (and including) order c^{-2}, such that the total given expansion order makes sense. We also recall that, as introduced in section 2.3, $\boldsymbol{\nabla}\times\boldsymbol{A}_{\text{tot.}}$ denotes the 'component-wise curl' of $\boldsymbol{A}_{\text{tot.}}$, which is a well-defined geometric operation (i. e. independent of coordinates) once we have introduced the background structures.

The internal-internal term of (4.4.39) was considered above in (4.4.38). The purely external term gives

$$
\begin{aligned}
L_{\text{em,ext.}} &= -\frac{\varepsilon_0 c^2}{4}\int \mathrm{d}^3\boldsymbol{x}\,\sqrt{-g}\,F_{\mu\nu}F^{\mu\nu}\\
&= \frac{\varepsilon_0}{2}\int \mathrm{d}^3\boldsymbol{x}\left[\left(1-(\gamma+1)\frac{\phi}{c^2}\right)\left((\partial_t\boldsymbol{A}^\perp)^2 + 2\partial_t\boldsymbol{A}^\perp\cdot\underbrace{\boldsymbol{\nabla}\phi_{\text{el.,ext.}}}_{\overset{(4.4.31)}{=}\mathrm{O}(c^{-2})}\right.\right.\\
&\qquad \left.\left. + \underbrace{(\boldsymbol{\nabla}\phi_{\text{el.,ext.}})^2}_{\overset{(4.4.31)}{=}\mathrm{O}(c^{-4})}\right) - c^2\left(1+(\gamma+1)\frac{\phi}{c^2}\right)(\boldsymbol{\nabla}\times\boldsymbol{A}^\perp)^2\right] + \mathrm{O}(c^{-4})\\
&\quad \text{(using P.I., (4.4.9))}\\
&= \frac{\varepsilon_0}{2}\int \mathrm{d}^3\boldsymbol{x}\left[\left(1-(\gamma+1)\frac{\phi}{c^2}\right)(\partial_t\boldsymbol{A}^\perp)^2\right.\\
&\qquad \left. - c^2\left(1+(\gamma+1)\frac{\phi}{c^2}\right)(\boldsymbol{\nabla}\times\boldsymbol{A}^\perp)^2\right] + \mathrm{O}(c^{-4}). \qquad (4.4.40)
\end{aligned}
$$

For the external-internal mixed term plus the interaction of the external potential with the current, we obtain

$$
\begin{aligned}
L_{\text{em,ext.-int.}} &= \int \mathrm{d}^3\boldsymbol{x}\, j^\mu A_\mu - \frac{\varepsilon_0 c^2}{2}\int \mathrm{d}^3\boldsymbol{x}\,\sqrt{-g}\,\mathcal{F}_{\mu\nu}F^{\mu\nu}\\
&= \int \mathrm{d}^3\boldsymbol{x}\,(\boldsymbol{j}\cdot\boldsymbol{A}^\perp - \rho\phi_{\text{el.,ext.}})\\
&\quad + \varepsilon_0\int \mathrm{d}^3\boldsymbol{x}\left[\left(1-(\gamma+1)\frac{\phi}{c^2}\right)(\partial_t\boldsymbol{\mathcal{A}}^\perp + \boldsymbol{\nabla}\phi_{\text{el.}})\cdot(\partial_t\boldsymbol{A}^\perp + \boldsymbol{\nabla}\phi_{\text{el.,ext.}})\right.\\
&\qquad \left. - c^2\left(1+(\gamma+1)\frac{\phi}{c^2}\right)(\boldsymbol{\nabla}\times\boldsymbol{\mathcal{A}}^\perp)\cdot(\boldsymbol{\nabla}\times\boldsymbol{A}^\perp)\right] + \mathrm{O}(c^{-4})
\end{aligned}
$$

$$
\begin{aligned}
&\text{(using (4.4.23), (4.4.31))} \\
&= \int \mathrm{d}^3\boldsymbol{x}\,(\boldsymbol{j}\cdot\boldsymbol{A}^\perp - \rho\phi_{\text{el.,ext.}}) \\
&\quad + \varepsilon_0 \int \mathrm{d}^3\boldsymbol{x} \bigg[(\partial_t \boldsymbol{\mathcal{A}}^\perp)\cdot(\partial_t \boldsymbol{A}^\perp) \\
&\quad - c^2\left(1+(\gamma+1)\frac{\phi}{c^2}\right)(\boldsymbol{\nabla}\times\boldsymbol{\mathcal{A}}^\perp)\cdot(\boldsymbol{\nabla}\times\boldsymbol{A}^\perp) \\
&\quad + \left(1-(\gamma+1)\frac{\phi}{c^2}\right)\boldsymbol{\nabla}\phi_{\text{el.}}\cdot\partial_t\boldsymbol{A}^\perp + \boldsymbol{\nabla}\phi_{\text{el.}}\cdot\boldsymbol{\nabla}\phi_{\text{el.,ext.}}\bigg] + \mathrm{O}(c^{-4}) \\
&\text{(using P.I., (4.4.9), (4.4.19a))} \\
&= \int \mathrm{d}^3\boldsymbol{x}\,\boldsymbol{j}\cdot\boldsymbol{A}^\perp + \varepsilon_0 \int \mathrm{d}^3\boldsymbol{x}\bigg[(\partial_t \boldsymbol{\mathcal{A}}^\perp)\cdot(\partial_t \boldsymbol{A}^\perp) \\
&\quad - c^2\left(1+(\gamma+1)\frac{\phi}{c^2}\right)(\boldsymbol{\nabla}\times\boldsymbol{\mathcal{A}}^\perp)\cdot(\boldsymbol{\nabla}\times\boldsymbol{A}^\perp)\bigg] \\
&\quad + \varepsilon_0 \int \mathrm{d}^3\boldsymbol{x}\,(\gamma+1)\,\phi_{\text{el.}}^{(0)}\frac{\boldsymbol{\nabla}\phi}{c^2}\cdot\partial_t\boldsymbol{A}^\perp + \mathrm{O}(c^{-4}).
\end{aligned}
\tag{4.4.41}
$$

Following appendix B of [SB18], we will neglect the second integral in this expression since it is related to formally diverging backreaction terms.

Adding the Lagrangians (4.4.38), (4.4.40) and (4.4.41), the total post-Newtonian electromagnetic Lagrangian (with the above-mentioned neglections following [SB18]) reads

$$
\begin{aligned}
L_{\text{em}} &= \frac{1}{2}\int \mathrm{d}^3\boldsymbol{x}\,(\boldsymbol{j}\cdot\boldsymbol{\mathcal{A}}^\perp - \rho\phi_{\text{el.}}) + \int \mathrm{d}^3\boldsymbol{x}\,\boldsymbol{j}\cdot\boldsymbol{A}^\perp \\
&\quad + \frac{\varepsilon_0}{2}\int \mathrm{d}^3\boldsymbol{x}\left[\left(1-(\gamma+1)\frac{\phi}{c^2}\right)(\partial_t\boldsymbol{A}^\perp)^2 - c^2\left(1+(\gamma+1)\frac{\phi}{c^2}\right)(\boldsymbol{\nabla}\times\boldsymbol{A}^\perp)^2\right] \\
&\quad + \varepsilon_0\int \mathrm{d}^3\boldsymbol{x}\,(\gamma+1)\,\phi_{\text{el.}}^{(0)}\frac{\boldsymbol{\nabla}\phi}{c^2}\cdot\partial_t\boldsymbol{A}^\perp + \mathrm{O}(c^{-4}).
\end{aligned}
\tag{4.4.42}
$$

We remind the reader that, as for the non-gravitational calculation discussed in section 4.2.1, $\boldsymbol{A}^\perp$ is treated as a given external field that appears in the Lagrangian, not a dynamical variable. Inserting the internal magnetic potential (4.4.23) and using the electric interaction integral (4.4.28) computed above, for the internal term we obtain (dropping infinite self-interaction terms)

$$
\begin{aligned}
\frac{1}{2}\int \mathrm{d}^3\boldsymbol{x}\,(\boldsymbol{j}\cdot\boldsymbol{\mathcal{A}}^\perp - \rho\phi_{\text{el.}}) &= -\frac{e_1e_2}{4\pi\varepsilon_0 r}\left(1+(\gamma+1)\frac{\phi(\boldsymbol{r}_1)+\phi(\boldsymbol{r}_2)}{2c^2}\right) \\
&\quad + \frac{e_1e_2}{8\pi\varepsilon_0c^2}\left[\frac{\dot{\boldsymbol{r}}_1\cdot\dot{\boldsymbol{r}}_2}{r} + \frac{(\dot{\boldsymbol{r}}_1\cdot\boldsymbol{r})(\dot{\boldsymbol{r}}_2\cdot\boldsymbol{r})}{r^3}\right] + \mathrm{O}(c^{-4}).
\end{aligned}
\tag{4.4.43}
$$

4.5. The total Hamiltonian including all interactions

In this section we collect all previous findings and combine them into the total Hamiltonian that characterises the dynamics of our two-particle system that is now also exposed to a non-trivial gravitational field. We will see that the Hamiltonian suffers various 'corrections' as compared to the gravity-free case, and that these terms acquire an intuitive interpretation if re-expressed in terms of the physical spacetime metric g.

4.5.1. Computation of the Hamiltonian

We will now compute the total Hamiltonian describing the atom in external electromagnetic and gravitational fields by repeating the calculation from section 4.3 while including the 'gravitational corrections' to electromagnetism obtained in section 4.4.

Comparing the gravitationally corrected electromagnetic Lagrangian as given by (4.4.42), (4.4.43) to the one without gravitational field ($\phi = 0$), we see that (at our order of approximation) the differences consist of new prefactors involving ϕ in the external electromagnetic term and the internal Coulomb interaction term, as well as an additional term involving the derivative $\boldsymbol{\nabla}\phi$ of the gravitational potential (last line of (4.4.43)). Thus, when calculating the Hamiltonian, we have to take care of these changes compared to the discussion of section 4.3.

The classical Hamiltonian

As explained in section 4.2.1, although the external field is not treated as a dynamical variable, when Legendre transforming the Lagrangian in order to compute a Hamiltonian we will add a term corresponding to the energy of the external field. We also use the notation $\boldsymbol{\Pi}^\perp$ for the 'would-be canonical momentum' conjugate to the external field (i.e. the canonical momentum if $\boldsymbol{A}^\perp$ were a dynamical variable). For our Lagrangian, this 'would-be canonical momentum' is

$$\begin{aligned}\boldsymbol{\Pi}^\perp &= \frac{\delta L_{\mathrm{em}}}{\delta(\partial_t \boldsymbol{A}^\perp)}\\ &= \varepsilon_0 \left(1 - (\gamma+1)\frac{\phi}{c^2}\right)\partial_t \boldsymbol{A}^\perp + \varepsilon_0(\gamma+1)\left(\phi_{\mathrm{el.}}^{(0)}\frac{\boldsymbol{\nabla}\phi}{c^2}\right)^\perp + \mathrm{O}(c^{-4}). \qquad (4.5.1)\end{aligned}$$

Inverting this, we get

$$\partial_t \boldsymbol{A}^\perp = \left(1 + (\gamma+1)\frac{\phi}{c^2}\right)\frac{\boldsymbol{\Pi}^\perp}{\varepsilon_0} - (\gamma+1)\left(\phi_{\mathrm{el.}}^{(0)}\frac{\boldsymbol{\nabla}\phi}{c^2}\right)^\perp + \mathrm{O}(c^{-4}). \qquad (4.5.2)$$

Expressing the first part of the external electromagnetic Lagrangian (4.4.40) in terms of this, we have

$$\begin{aligned}
&\frac{\varepsilon_0}{2}\int \mathrm{d}^3\boldsymbol{x}\left(1-(\gamma+1)\frac{\phi}{c^2}\right)(\partial_t \boldsymbol{A}^\perp)^2 \\
&\quad= \frac{\varepsilon_0}{2}\int \mathrm{d}^3\boldsymbol{x}\left(\frac{\boldsymbol{\Pi}^\perp}{\varepsilon_0}-(\gamma+1)\,\phi^{(0)}_{\text{el.}}\frac{\boldsymbol{\nabla}\phi}{c^2}\right)\cdot(\partial_t \boldsymbol{A}^\perp)+\mathrm{O}(c^{-4}) \\
&\quad= \frac{\varepsilon_0}{2}\int \mathrm{d}^3\boldsymbol{x}\left(1+(\gamma+1)\frac{\phi}{c^2}\right)(\boldsymbol{\Pi}^\perp/\varepsilon_0)^2-\int \mathrm{d}^3\boldsymbol{x}\,(\gamma+1)\,\phi^{(0)}_{\text{el.}}\frac{\boldsymbol{\nabla}\phi}{c^2}\cdot\boldsymbol{\Pi}^\perp+\mathrm{O}(c^{-4}).
\end{aligned} \tag{4.5.3}$$

Furthermore, we have

$$\begin{aligned}
\int \mathrm{d}^3\boldsymbol{x}\,\boldsymbol{\Pi}^\perp\cdot\partial_t\boldsymbol{A}^\perp &= \varepsilon_0\int \mathrm{d}^3\boldsymbol{x}\left(1+(\gamma+1)\frac{\phi}{c^2}\right)(\boldsymbol{\Pi}^\perp/\varepsilon_0)^2 \\
&\quad-\int \mathrm{d}^3\boldsymbol{x}\,(\gamma+1)\,\phi^{(0)}_{\text{el.}}\frac{\boldsymbol{\nabla}\phi}{c^2}\cdot\boldsymbol{\Pi}^\perp+\mathrm{O}(c^{-4}).
\end{aligned} \tag{4.5.4}$$

Thus, the Hamiltonian for the external electromagnetic field and the external-internal interaction is

$$\begin{aligned}
H_{\text{em,ext.,ext.-int.}} &= \int \mathrm{d}^3\boldsymbol{x}\,\boldsymbol{\Pi}^\perp\cdot\partial_t\boldsymbol{A}^\perp - L_{\text{em,ext.}} - L_{\text{em,ext.-int.}} \\
&= \int \mathrm{d}^3\boldsymbol{x}\,\boldsymbol{\Pi}^\perp\cdot\partial_t\boldsymbol{A}^\perp - L_{\text{em,ext.}} \\
&\quad-\int \mathrm{d}^3\boldsymbol{x}\,\boldsymbol{j}\cdot\boldsymbol{A}^\perp-\varepsilon_0\int \mathrm{d}^3\boldsymbol{x}\,(\gamma+1)\,\phi^{(0)}_{\text{el.}}\frac{\boldsymbol{\nabla}\phi}{c^2}\cdot\underbrace{\partial_t\boldsymbol{A}^\perp}_{=\boldsymbol{\Pi}^\perp/\varepsilon_0+\mathrm{O}(c^{-2})}+\mathrm{O}(c^{-4}) \\
&= \frac{\varepsilon_0}{2}\int \mathrm{d}^3\boldsymbol{x}\left(1+(\gamma+1)\frac{\phi}{c^2}\right)\left[(\boldsymbol{\Pi}^\perp/\varepsilon_0)^2+c^2(\boldsymbol{\nabla}\times\boldsymbol{A}^\perp)^2\right] \\
&\quad-\int \mathrm{d}^3\boldsymbol{x}\,\boldsymbol{j}\cdot\boldsymbol{A}^\perp-\int \mathrm{d}^3\boldsymbol{x}\,(\gamma+1)\,\phi^{(0)}_{\text{el.}}\frac{\boldsymbol{\nabla}\phi}{c^2}\cdot\boldsymbol{\Pi}^\perp+\mathrm{O}(c^{-4}).
\end{aligned} \tag{4.5.5}$$

When including the gravitational corrections to electromagnetism, the final total classical Hamiltonian thus will differ from the one without these corrections, as given by (4.3.3) and ([SB18].12⋆), in the following points:

- The external 'field energy' $\frac{\varepsilon_0}{2}\int \mathrm{d}^3\boldsymbol{x}\left[(\boldsymbol{\Pi}^\perp/\varepsilon_0)^2+c^2(\boldsymbol{\nabla}\times\boldsymbol{A}^\perp)^2\right]$ gains a prefactor $\left(1+(\gamma+1)\frac{\phi}{c^2}\right)$,
- the Coulomb term gains a prefactor $\left(1+(\gamma+1)\frac{\phi(\boldsymbol{r}_1)+\phi(\boldsymbol{r}_2)}{2c^2}\right)$, and

- there is an additional term

$$-\int \mathrm{d}^3\boldsymbol{x}\,(\gamma+1)\,\phi_{\text{el.}}^{(0)}\frac{\boldsymbol{\nabla}\phi}{c^2}\cdot\boldsymbol{\Pi}^{\perp}. \tag{4.5.6}$$

Canonical quantisation, PZW transformation, and introduction of centre of mass coordinates

We can now canonically quantise this classical Hamiltonian and perform the PZW transformation precisely as in the case without the gravitational corrections to electromagnetism – we just have to see how the correction terms transform. The resulting final multipolar Hamiltonian differs from the one without these corrections, as given by (4.3.4) and ([SB18].23⋆), in the following points:

- The transformed external 'field energy' $\frac{\varepsilon_0}{2}\int \mathrm{d}^3\boldsymbol{x}\left[\frac{(\tilde{\boldsymbol{\Pi}}^{\perp}+\boldsymbol{\mathcal{P}}_d^{\perp})^2}{\varepsilon_0^2}+c^2(\boldsymbol{\nabla}\times\boldsymbol{A}^{\perp})^2\right]$ gains a prefactor $\left(1+(\gamma+1)\frac{\phi}{c^2}\right)$,
- the Coulomb term gains a prefactor $\left(1+(\gamma+1)\frac{\phi(\boldsymbol{r}_1)+\phi(\boldsymbol{r}_2)}{2c^2}\right)$, and
- there are additional terms

$$-\int \mathrm{d}^3\boldsymbol{x}\,(\gamma+1)\,\phi_{\text{el.}}^{(0)}\frac{\boldsymbol{\nabla}\phi}{c^2}\cdot(\tilde{\boldsymbol{\Pi}}^{\perp}+\boldsymbol{\mathcal{P}}_d^{\perp}). \tag{4.5.7}$$

For the Coulomb term, expanding ϕ to linear order, we have

$$\begin{aligned}\phi(\boldsymbol{r}_1)+\phi(\boldsymbol{r}_2)&=2\phi(\boldsymbol{R})+(\boldsymbol{r}_1-\boldsymbol{R}+\boldsymbol{r}_2-\boldsymbol{R})\cdot\boldsymbol{\nabla}\phi(\boldsymbol{R})\\&=2\phi(\boldsymbol{R})+\frac{m_2-m_1}{M}\boldsymbol{r}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{R}).\end{aligned} \tag{4.5.8}$$

Using this, we can rewrite the corrected Coulomb term as

$$\begin{aligned}-\left(1+(\gamma+1)\frac{\phi(\boldsymbol{r}_1)+\phi(\boldsymbol{r}_2)}{2c^2}\right)\frac{e^2}{4\pi\varepsilon_0 r}&=-\frac{e^2}{4\pi\varepsilon_0 r}\left(1+(\gamma+1)\frac{\phi(\boldsymbol{R})}{c^2}\right)\\&\quad-\frac{\gamma+1}{c^2}\frac{e^2}{8\pi\varepsilon_0 r}\frac{m_2-m_1}{M}\boldsymbol{r}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{R})\end{aligned} \tag{4.5.9}$$

in terms of centre of mass and relative coordinates.

The total Hamiltonian

Putting everything together, we arrive at the total Hamiltonian describing our simple atomic system in external electromagnetic and post-Newtonian gravitational fields. Here it is, in its full glory:

$$H_{[\mathrm{com}],\mathrm{final}} = H_{\mathrm{C,final}} + H_{\mathrm{A,final}} + H_{\mathrm{AL,final}} + H_{\mathrm{L,final}} + H_{\mathrm{X}} + H_{\mathrm{deriv,new}} + \mathrm{O}(c^{-4}) \tag{4.5.10a}$$

$$\begin{aligned} H_{\mathrm{C,final}} = {} & \frac{\boldsymbol{P}^2}{2M}\left[1 - \frac{1}{Mc^2}\left(\frac{\boldsymbol{p_r}^2}{2\mu} - \frac{e^2}{4\pi\varepsilon_0 r}\right)\right] + \left[M + \frac{1}{c^2}\left(\frac{\boldsymbol{p_r}^2}{2\mu} - \frac{e^2}{4\pi\varepsilon_0 r}\right)\right]\phi(\boldsymbol{R}) \\ & - \frac{\boldsymbol{P}^4}{8M^3c^2} + \frac{2\gamma+1}{2Mc^2}\boldsymbol{P}\cdot\phi(\boldsymbol{R})\boldsymbol{P} + (2\beta-1)\frac{M\phi(\boldsymbol{R})^2}{2c^2} \end{aligned} \tag{4.5.10b}$$

$$\begin{aligned} H_{\mathrm{A,final}} = {} & \left(1 + 2\gamma\frac{\phi(\boldsymbol{R})}{c^2}\right)\frac{\boldsymbol{p_r}^2}{2\mu} - \left(1 + \gamma\frac{\phi(\boldsymbol{R})}{c^2}\right)\frac{e^2}{4\pi\varepsilon_0 r} \\ & - \frac{m_1^3 + m_2^3}{M^3}\frac{\boldsymbol{p_r}^4}{8\mu^3c^2} - \frac{e^2}{4\pi\varepsilon_0}\frac{1}{2\mu Mc^2}\left(\boldsymbol{p_r}\cdot\frac{1}{r}\boldsymbol{p_r} + \boldsymbol{p_r}\cdot\boldsymbol{r}\frac{1}{r^3}\boldsymbol{r}\cdot\boldsymbol{p_r}\right) \\ & - \frac{2\gamma+1}{2c^2}\frac{m_1 - m_2}{m_1 m_2}\boldsymbol{p_r}\cdot(\boldsymbol{r}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{R}))\boldsymbol{p_r} - \frac{\gamma+1}{c^2}\frac{e^2}{8\pi\varepsilon_0 r}\frac{m_2 - m_1}{M}\boldsymbol{r}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{R}) \end{aligned} \tag{4.5.10c}$$

$$\begin{aligned} H_{\mathrm{AL,final}} = {} & \left(1 + (\gamma+1)\frac{\phi(\boldsymbol{R})}{c^2}\right)\frac{\tilde{\boldsymbol{\Pi}}^{\perp}(\boldsymbol{R})}{\varepsilon_0}\cdot\boldsymbol{d} + \frac{1}{2M}\{\boldsymbol{P}\cdot[\boldsymbol{d}\times\boldsymbol{B}(\boldsymbol{R})] + \mathrm{H.c.}\} \\ & - \frac{m_1 - m_2}{4m_1 m_2}\{\boldsymbol{p_r}\cdot[\boldsymbol{d}\times\boldsymbol{B}(\boldsymbol{R})] + \mathrm{H.c.}\} \\ & + \frac{1}{8\mu}(\boldsymbol{d}\times\boldsymbol{B}(\boldsymbol{R}))^2 + \frac{1}{2\varepsilon_0}\int \mathrm{d}^3\boldsymbol{x}\left(1 + (\gamma+1)\frac{\phi}{c^2}\right)\boldsymbol{\mathcal{P}}_d^{\perp\,2}(\boldsymbol{x},t) \\ & - \int \mathrm{d}^3\boldsymbol{x}\,(\gamma+1)\,\phi_{\mathrm{el.}}^{(0)}\frac{\boldsymbol{\nabla}\phi}{c^2}\cdot(\tilde{\boldsymbol{\Pi}}^{\perp} + \boldsymbol{\mathcal{P}}_d^{\perp}) \end{aligned} \tag{4.5.10d}$$

$$H_{\mathrm{L,final}} = \frac{\varepsilon_0}{2}\int \mathrm{d}^3\boldsymbol{x}\left(1 + (\gamma+1)\frac{\phi}{c^2}\right)\left[(\tilde{\boldsymbol{\Pi}}^{\perp}/\varepsilon_0)^2 + c^2(\boldsymbol{\nabla}\times\boldsymbol{A}^{\perp})^2\right] \tag{4.5.10e}$$

$$\begin{aligned} H_{\mathrm{X}} = {} & -\frac{(\boldsymbol{P}\cdot\boldsymbol{p_r})^2}{2M^2\mu c^2} + \frac{e^2}{4\pi\varepsilon_0 r}\frac{(\boldsymbol{P}\cdot\boldsymbol{r}/r)^2}{2M^2c^2} \\ & + \frac{m_1 - m_2}{2\mu M^2c^2}\left\{(\boldsymbol{P}\cdot\boldsymbol{p_r})\boldsymbol{p_r}^2/\mu - \frac{e^2}{8\pi\varepsilon_0}\left[\frac{1}{r}\boldsymbol{P}\cdot\boldsymbol{p_r} + \frac{1}{r^3}(\boldsymbol{P}\cdot\boldsymbol{r})(\boldsymbol{r}\cdot\boldsymbol{p_r}) + \mathrm{H.c.}\right]\right\} \end{aligned} \tag{4.5.10f}$$

$$H_{\mathrm{deriv,new}} = \frac{2\gamma+1}{2Mc^2}[\boldsymbol{P}\cdot(\boldsymbol{r}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{R}))\boldsymbol{p_r} + \mathrm{H.c.}] \tag{4.5.10g}$$

Here, we have included the term $-\gamma \frac{1}{c^2} \frac{e^2}{4\pi\varepsilon_0 r} \phi(\boldsymbol{R})$ (from the 'corrections' to the Coulomb term) into $H_{\mathrm{A,final}}$ (instead of into $H_{\mathrm{C,final}}$) since it can be combined with the original Coulomb term from H_{A} into

$$- \frac{e^2}{4\pi\varepsilon_0 r} \left(1 + \gamma \frac{\phi(\boldsymbol{R})}{c^2}\right) = - \frac{e^2}{4\pi\varepsilon_0 \sqrt{{}^{(3)}g_{\boldsymbol{R}}(\boldsymbol{r}, \boldsymbol{r})}}\,, \tag{4.5.11}$$

i.e. a Coulomb term expressed with the correct, metric relative distance.

To correctly interpret the atom–light interaction Hamiltonian (4.5.10d), one has to keep in mind that the field variables $\tilde{\boldsymbol{\Pi}}^{\perp} = \boldsymbol{\Pi}^{\perp} - \boldsymbol{\mathcal{P}}^{\perp}$ and $\boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}^{\perp}$ appearing in it do not refer to an orthonormal frame in the physical spacetime metric g in the presence of gravitational fields, but are related to components of the electromagnetic field tensor in the *coordinate* frame – or, more geometrically speaking, to an inertial frame with respect to the background Minkowski metric. This issue will be discussed in more detail in section 4.5.3.

Since the cross terms H_{X} are the same as in [SB18], we could now introduce new canonical variables $\boldsymbol{Q}, \boldsymbol{q}, \boldsymbol{p}$ literally as in ([SB18].26) to eliminate these cross terms. Since the gravitational correction terms are of order $\mathrm{O}(c^{-2})$, for them this canonical transformation would just amount to the replacements $\boldsymbol{R} \to \boldsymbol{Q}, \boldsymbol{r} \to \boldsymbol{q}, \boldsymbol{p}_{\boldsymbol{r}} \to \boldsymbol{p}$ at our order of approximation. Since it will not alter the following discussion, we will not perform this coordinate change in order to avoid adding an extra layer of potentially confusing notation.

4.5.2. The system as a composite point particle

We now take another look at the central and the internal Hamiltonian (4.5.10b), (4.5.10c), where we rewrite the latter in the form

$$\begin{aligned} H_{\mathrm{A,final}} = {} & \frac{{}^{(3)}g_{\boldsymbol{R}}^{-1}(\boldsymbol{p}_{\boldsymbol{r}}, \boldsymbol{p}_{\boldsymbol{r}})}{2\mu} - \frac{e^2}{4\pi\varepsilon_0 \sqrt{{}^{(3)}g_{\boldsymbol{R}}(\boldsymbol{r}, \boldsymbol{r})}} \\ & - \frac{m_1^3 + m_2^3}{M^3} \frac{\boldsymbol{p}_{\boldsymbol{r}}^4}{8\mu^3 c^2} - \frac{e^2}{4\pi\varepsilon_0} \frac{1}{2\mu M c^2} \left(\boldsymbol{p}_{\boldsymbol{r}} \cdot \frac{1}{r} \boldsymbol{p}_{\boldsymbol{r}} + \boldsymbol{p}_{\boldsymbol{r}} \cdot \boldsymbol{r} \frac{1}{r^3} \boldsymbol{r} \cdot \boldsymbol{p}_{\boldsymbol{r}}\right) \\ & - \frac{2\gamma + 1}{2c^2} \frac{m_1 - m_2}{m_1 m_2} \boldsymbol{p}_{\boldsymbol{r}} \cdot (\boldsymbol{r} \cdot \boldsymbol{\nabla}\phi(\boldsymbol{R})) \boldsymbol{p}_{\boldsymbol{r}} - \frac{\gamma + 1}{c^2} \frac{e^2}{8\pi\varepsilon_0 r} \frac{m_2 - m_1}{M} \boldsymbol{r} \cdot \boldsymbol{\nabla}\phi(\boldsymbol{R}) \end{aligned} \tag{4.5.12}$$

by combining the gravitational correction terms which do not involve the potential derivative $\boldsymbol{\nabla}\phi$ into metrically defined kinetic energy and Coulomb terms as in (4.3.13), (4.5.11).

Now comparing the central Hamiltonian $H_{\mathrm{C,final}}$ (4.5.10b) to the Hamiltonian of a single point particle of mass m in the PPN metric,

$$H_{\mathrm{point}}(\boldsymbol{P}, \boldsymbol{R}; m) = \frac{\boldsymbol{P}^2}{2m} + m\phi(\boldsymbol{R}) - \frac{\boldsymbol{P}^4}{8m^3c^2} + \frac{2\gamma+1}{2mc^2}\boldsymbol{P}\cdot\phi(\boldsymbol{R})\boldsymbol{P} + (2\beta-1)\frac{m\phi(\boldsymbol{R})^2}{2c^2}\,, \tag{4.5.13}$$

we see that the central Hamiltonian has, up to (and including) $\mathrm{O}(c^{-2})$, exactly this form, with the mass m replaced by $M + \frac{H_{\mathrm{A,final}}}{c^2}$,

$$H_{\mathrm{C,final}} = H_{\mathrm{point}}\left(\boldsymbol{P}, \boldsymbol{R}; M + \frac{H_{\mathrm{A,final}}}{c^2}\right), \tag{4.5.14}$$

as could be naively expected from mass–energy equivalence. Thus, starting from first principles, we have shown that *the system behaves as a 'composite point particle' whose (inertial as well as gravitational) mass is comprised of the rest masses of the constituent particles as well as the internal energy.*

Note that this conclusion depends on the identification of terms as being 'kinetic' and 'interaction' energies, which in turn depends on the metric structure in their expressions. Had we not rewritten the internal kinetic energy (4.3.13) and the Coulomb interaction (4.5.11) in terms of the physical metric g, but included only the corresponding terms $\frac{\boldsymbol{p}_r^2}{2\mu}$ and $-\frac{e^2}{4\pi\varepsilon_0 r}$ with respect to the background metric into the internal Hamiltonian, the above conclusion could not have resulted. Rather, having additional terms in the central Hamiltonian, to obtain it in a 'composite particle' point of view we would have had to replace the inertial mass in (4.5.13) by $M + H_{\mathrm{A}}/c^2$ and the gravitational mass by $M + (2\gamma+1)\frac{\boldsymbol{p}_r^2}{2\mu c^2} - (\gamma+1)\frac{e^2}{4\pi\varepsilon_0 rc^2} = M + \frac{H_{\mathrm{A}}}{c^2} + \gamma\left(2\frac{\boldsymbol{p}_r^2}{2\mu c^2} - \frac{e^2}{4\pi\varepsilon_0 rc^2}\right)$, which one could have erroneously interpreted as a violation of some naive form of the weak equivalence principle. But, clearly, such a conclusion would be premature, for it is based on the identification of terms – like inertial and gravitational mass – that is itself ambiguous. That ambiguity is here seen as a dependence on the background structure, which is used to define distances of positions and squares of momenta. Once these quantities are measured with the physical metric g, ambiguities and apparent conflicts with naive expectations disappear. That point has also been made in [ZRP19].

The quantities $\vec{p}'^2$ and r' entering the Hamiltonian in [ZRP19, eq. (18)], which are, in the language of [ZRP19], the square of the internal momentum and the distance 'in the CM rest frame', are nothing but the geometric expressions ${}^{(3)}g_{\boldsymbol{R}}^{-1}(\boldsymbol{p}_r, \boldsymbol{p}_r)$ and $\sqrt{{}^{(3)}g_{\boldsymbol{R}}(\boldsymbol{r}, \boldsymbol{r})}$ from above, measured using the physical metric of space. The internal Hamiltonian (4.5.12) thus consists of kinetic and Coulomb interaction energies in terms of the physical geometry, in agreement with the expressions from [ZRP19], as well as the expected special-relativistic and 'Darwin' corrections, and terms involving the gravitational potential's derivative[9].

[9]Since all these corrections are themselves of order $1/c^2$, the deviations of the physical from the flat

4.5.3. The electromagnetic expressions in terms of components with respect to orthonormal frames

The expressions derived above in (4.5.10) include components of the external electromagnetic field with respect to coordinates which, albeit not chosen arbitrarily, have no direct metric significance. We recall that we used coordinates that are adapted to the background structure (η, u), in the sense that $u = \partial/\partial t$ and $\eta = \eta_{\mu\nu}\,\mathrm{d}x^\mu \otimes \mathrm{d}x^\nu$ with $(\eta_{\mu\nu}) = \mathrm{diag}(-1, 1, 1, 1)$. The corresponding local reference frames $(\partial_\mu = \partial/\partial x^\mu)_{\mu=0,1,2,3}$ are orthonormal with respect to the background metric η, but not with respect to the physical metric g.

In this section we will re-express our findings in terms of components with respect to g-orthonormal frames, which we will call the 'physical components', as opposed to the 'coordinate components' used so far. We stress that, despite this terminology, there is nothing wrong or 'unphysical' with representing fields in terms of components of non-orthonormal bases, as long as the metric properties are spelled out at the same time. Yet it is clearly convenient to be able to read off metric properties, which bear direct metric significance, from the expressions involving the components alone, without at the same time having to recall the values of the metric components as well.

Electromagnetic quantities in non-orthonormal and orthonormal frames

At first, we will discuss the meaning of several 'electromagnetic quantities' in non-orthonormal and orthonormal frames in general, before specialising to the case of our PPN metric and considering the terms in our Hamiltonian. Suppose that we are given our usual 'background' coordinate system (x^0, x^a), that is possibly non-orthonormal with respect to the physical spacetime metric g, as well as a time- and space-oriented orthonormal frame / 'tetrad' $(\mathrm{e}_{\underline{\mu}})_{\underline{\mu}=0,1,2,3}$ for the physical metric, where from now on underlined indices refer to components with respect to the tetrad. We write the tetrad fields in terms of the coordinate basis fields, and vice versa, as

$$\mathrm{e}_{\underline{\mu}} = \mathrm{e}^{\nu}_{\underline{\mu}}\,\partial_\nu\,, \quad \partial_\mu = \mathrm{e}^{\underline{\nu}}_{\mu}\,\mathrm{e}_{\underline{\nu}}\,, \tag{4.5.15}$$

where the matrices of coefficients $(\mathrm{e}^{\nu}_{\underline{\mu}})$ and $(\mathrm{e}^{\underline{\nu}}_{\mu})$ are inverses of each other. Since the tetrad is orthonormal, i.e. the tetrad components $g_{\underline{\mu\nu}}$ of the metric are numerically equal to the components $\eta_{\mu\nu}$ of the Minkowski metric in a Lorentz frame, we can express the coordinate components of the metric as

$$g_{\mu\nu} = \mathrm{e}^{\underline{\rho}}_{\mu}\,\mathrm{e}^{\underline{\sigma}}_{\nu}\,g_{\underline{\rho\sigma}} = \sum_{\rho,\sigma=0}^{3} \mathrm{e}^{\underline{\rho}}_{\mu}\,\mathrm{e}^{\underline{\sigma}}_{\nu}\,\eta_{\rho\sigma}\,. \tag{4.5.16}$$

metric do not enter here.

We make the further assumption that at any point, time and space as defined by both bases be the same, i.e. that

$$\mathrm{span}\{e_0\} = \mathrm{span}\{\partial_0\}, \quad \mathrm{span}\{\mathrm{e}_1, \mathrm{e}_2, \mathrm{e}_3\} = \mathrm{span}\{\partial_1, \partial_2, \partial_3\}, \tag{4.5.17}$$

i.e. that the coefficients $\mathrm{e}^{a}_{\underline{0}}, \mathrm{e}^{0}_{\underline{a}}, \mathrm{e}^{\underline{0}}_{a}, \mathrm{e}^{\underline{a}}_{0}, g_{0a}, g^{0a}$ all vanish (which will in our later application to the electromagnetic Hamiltonian be satisfied to our order of expansion). This also implies that $\sqrt{-g_{00}} = \mathrm{e}^{\underline{0}}_{0} = 1/\,\mathrm{e}^{0}_{\underline{0}}$.

Now we can consider how electromagnetic quantities are related to the components of the field tensor in the two different frames. The electric and magnetic field components with respect to the tetrad (which we call, as introduced above, the 'physical' field components) are

$$E_{\mathrm{phys.}\underline{a}} = cF_{\underline{a0}}\,, \quad B^{\underline{a}}_{\mathrm{phys.}} = {}^{(3)}\hat{\varepsilon}^{\underline{abc}} F_{\underline{bc}} \tag{4.5.18}$$

in terms of the tetrad components of the field tensor, where ${}^{(3)}\hat{\varepsilon}^{\underline{abc}}$ is the three-dimensional totally antisymmetric symbol. Note that although written in component form, these formulae have an invariant geometric meaning that depends only on being given the time direction $\mathrm{span}\{\partial_0\} = \mathrm{span}\{\mathrm{e}_0\}$ and the (physical) metric g: the electric field is simply the spatial[10] one-form obtained by inserting the unit future-pointing time direction vector e_0 into the two-form F (in its second argument), projecting onto space, and multiplying with c. Considering the magnetic field, we recall the well-known fact that we can view ${}^{(3)}\hat{\varepsilon}^{\underline{abc}}$ as the components of a spatial tensor density ${}^{(3)}\hat{\varepsilon}$ of weight[11] $+1$ which is defined by demanding that its components in *any* positively oriented frame are given by the totally antisymmetric symbol. Thus, the magnetic field is a contraction of this tensor density ${}^{(3)}\hat{\varepsilon}$ and the (spatially projected) field tensor (which is a proper tensor, i.e. a density of weight 0), i.e. itself a spatial vector density of weight $+1$.

This means that what one might call the 'coordinate components' of the magnetic field, namely the expressions

$$B^{a}_{\mathrm{coord.}} = {}^{(3)}\hat{\varepsilon}^{abc} F_{bc} \tag{4.5.19}$$

where ${}^{(3)}\hat{\varepsilon}^{abc}$ is the totally antisymmetric symbol, are in fact the components with respect to the coordinate frame of *the same* geometric object as for the 'physical components', namely the above tensor density. Thus, the components are related by the usual transformation formula for tensor densities, i.e.

$$B^{\underline{a}}_{\mathrm{phys.}} = \det(\mathrm{e}^{d}_{\underline{c}}) \cdot \mathrm{e}^{\underline{a}}_{b}\, B^{b}_{\mathrm{coord.}} = \frac{1}{\sqrt{{}^{(3)}g}}\, \mathrm{e}^{\underline{a}}_{b}\, B^{b}_{\mathrm{coord.}}\,, \tag{4.5.20}$$

[10] Here 'spatial' means geometric objects (i.e. tensor densities) defined on the 'spatial' submanifolds $x^0 = \text{const.}$, which integrate the spatial distribution $\mathrm{span}\{\mathrm{e}_1, \mathrm{e}_2, \mathrm{e}_3\} = \mathrm{span}\{\partial_1, \partial_2, \partial_3\}$.

[11] A more well-known fact is probably that the *covariant* totally antisymmetric symbol is a tensor density of weight -1; that the contravariant symbol may be considered a density of weight $+1$ one sees in exactly analogous fashion.

where ${}^{(3)}g$ denotes the determinant of the matrix of coordinate components of the spatial metric. Note that due to the numerical identity ${}^{(3)}\hat{\varepsilon}^{abc} = {}^{(3)}\varepsilon^{abc}$, where ${}^{(3)}\varepsilon^{abc}$ are the 'index-raised' components of the background spatial volume form as introduced in section 2.3, the components $B^a_{\text{coord.}}$ are, in fact, numerically equal to the components of the 'three-vector' $\boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}^{\perp}$ used in the previous sections (although we treated $\boldsymbol{B}$ as a different geometric object there, namely as a spatial vector field instead of a spatial vector field density). The interpretation of the magnetic field as a vector density also goes nicely with an intuitive point of view, namely that of the field representing the spatial density of magnetic field lines.

Expressing the electric field's tetrad components in terms of the coordinate components of the field tensor, we directly obtain

$$E_{\text{phys.}\underline{a}} = \mathrm{e}^b_{\underline{a}}\, \mathrm{e}^0_{\underline{0}}\, cF_{b0} = \frac{1}{\sqrt{-g_{00}}}\, \mathrm{e}^b_{\underline{a}}\, cF_{b0} \; . \tag{4.5.21}$$

One could interpret $\frac{1}{\sqrt{-g_{00}}} cF_{b0} =: E_{\text{coord.}b}$ as the 'coordinate components' of the electric field (interpreted as a spatial one-form as discussed above); however, we will not make much use of this notation.[12]

Next, we will consider electric dipole moments and (electric) polarisation. Imagining an ideal dipole in the usual way as arising in a limit process from two separated opposite point charges getting closer and closer, with their respective charges growing accordingly, the resulting dipole moment is to be a proper spatial vector (and not a density of non-zero weight): its magnitude is an invariant (i. e. frame-independent) quantity, namely the product of charge and distance of the two particles, held constant in the limit process, and its direction is the limit of the direction 'from one particle to

[12]In index-free notation, we can express the electric and magnetic fields as follows. The electric field is

$$E = -c\,\iota_{\mathrm{e}_{\underline{0}}} F$$

where ι denotes the interior product of a vector field and a differential form, i.e. insertion of the vector field into the *first* argument of the form. Note that E is spatial due to the antisymmetry of F.

The magnetic field can be expressed as

$$B = {}^{(3)}\widetilde{\mathrm{vol}} \cdot \left[{}^{(3)}\tilde{*} \left(\mathrm{Pr}^{\perp}(F) \right) \right]^{\tilde{\sharp}} .$$

The objects occurring in this formula are the following: $\mathrm{Pr}^{\perp}$ denotes the orthogonal projection map onto three-space $\mathrm{span}\{\mathrm{e}_{\underline{0}}\}^{\perp}$, extended to arbitrary tensors. The operator ${}^{(3)}\tilde{*}$ is the spatial Hodge star with respect to the physical spatial metric ${}^{(3)}g$. A superscript $\tilde{\sharp}$ denotes the natural isomorphism from spatial one-forms to spatial vector fields induced by the physical spatial metric, i.e. ${}^{(3)}g(\alpha^{\tilde{\sharp}}, \cdot) = \alpha$. Finally, ${}^{(3)}\widetilde{\mathrm{vol}}$ denotes the spatial 'volume density', i.e. the spatial scalar density whose value in any frame is the ${}^{(3)}g$-volume of the parallelepiped spanned by the frame's vectors. (The value of ${}^{(3)}\widetilde{\mathrm{vol}}$ is given by the square root of the determinant of the matrix of ${}^{(3)}g$'s components in the respective frame.)

the other'. Therefore, when a dipole moment has coordinate components $d^a_{\text{coord.}}$, its tetrad components are simply

$$d^{\underline{a}}_{\text{phys.}} = \mathrm{e}^{\underline{a}}_b \, d^b_{\text{coord.}} \,. \tag{4.5.22}$$

Now, since a polarisation is simply a density of dipole moment per spatial volume, the natural geometric perspective is that polarisation is a spatial vector density field. Thus a polarisation field with coordinate components $\mathcal{P}^a_{\text{coord.}}$ has tetrad components

$$\mathcal{P}^{\underline{a}}_{\text{phys.}} = \det(\mathrm{e}^d_{\underline{c}}) \cdot \mathrm{e}^{\underline{a}}_b \, \mathcal{P}^b_{\text{coord.}} = \frac{1}{\sqrt{^{(3)}g}} \mathrm{e}^{\underline{a}}_b \, \mathcal{P}^b_{\text{coord.}} \,. \tag{4.5.23}$$

Finally, we turn to the electric displacement field. In vacuum, it has the interpretation of electric flux density, with the only contribution to its value coming from the electric field times ε_0. However, the displacement is to be a vector *density*, so one has to identify the electric field spatial one-form with the corresponding vector field via the metric ('index raising') and consider the density that is metrically associated to this. In a medium, the displacement field is the sum of this vacuum displacement and the polarisation, i.e. we have

$$D^a_{\text{coord.}} = \varepsilon_0 \, {}^{(3)}g^{ab} E_{\text{coord.}b} \cdot \sqrt{^{(3)}g} + \mathcal{P}^a_{\text{coord.}} \,. \tag{4.5.24}$$

In tetrad components, it takes the form

$$D^{\underline{a}}_{\text{phys.}} = \varepsilon_0 \, {}^{(3)}g^{\underline{ab}} E_{\text{phys.}\underline{b}} + \mathcal{P}^{\underline{a}}_{\text{phys.}} \,, \tag{4.5.25}$$

where ${}^{(3)}g^{\underline{ab}}$ are the tetrad components of the physical spatial metric, which are numerically equal to the Kronecker delta δ^{ab}.

Application to the Hamiltonian

We will now rewrite the parts of the total Hamiltonian (4.5.10) in which the external electromagnetic field appears in terms of electromagnetic quantities in an orthonormal tetrad, as discussed above. Due to the form of the Eddington–Robertson PPN metric, in order to obtain a tetrad, to our order of approximation we simply need to divide each of the coordinate basis vectors ∂_μ by the square root of the modulus of $g_{\mu\mu}$ (no summation):

$$\mathrm{e}_{\underline{0}} = \frac{1}{\sqrt{-g_{00}}} \partial_0 = \left(1 - \frac{\phi}{c^2}\right) \partial_0 \tag{4.5.26a}$$

$$\mathrm{e}_{\underline{a}} = \frac{1}{\sqrt{g_{aa}}} \partial_a = \left(1 + \gamma \frac{\phi}{c^2}\right) \partial_a \tag{4.5.26b}$$

Inserting this explicit form of the tetrad, the relevant equations from above relating the tetrad components of electromagnetic quantities to their coordinate components attain the following numerical forms:

$$B^{\underline{a}}_{\text{phys.}} = \left(1 + 2\gamma\frac{\phi}{c^2}\right) B^a_{\text{coord.}} \tag{4.5.27a}$$

$$d^{\underline{a}}_{\text{phys.}} = \left(1 - \gamma\frac{\phi}{c^2}\right) d^a_{\text{coord.}} \tag{4.5.27b}$$

$$\mathcal{P}^{\underline{a}}_{\text{phys.}} = \left(1 + 2\gamma\frac{\phi}{c^2}\right) \mathcal{P}^a_{\text{coord.}} \tag{4.5.27c}$$

$$D^{\underline{a}}_{\text{phys.}} = \varepsilon_0 \left(1 + (\gamma - 1)\frac{\phi}{c^2}\right) cF_{a0} + \left(1 + 2\gamma\frac{\phi}{c^2}\right) \mathcal{P}^a_{\text{coord.}} \tag{4.5.27d}$$

Comparing (4.5.27d) to the form (4.5.1) of the 'would-be canonical field momentum' $\mathbf{\Pi}^\perp$ and its relation $\tilde{\mathbf{\Pi}}^\perp = \mathbf{\Pi}^\perp - \boldsymbol{\mathcal{P}}^\perp$ to the 'would-be field momentum' after the PZW transformation, we can relate the coordinate components of the latter to the tetrad components of the displacement field by

$$D^{\perp\,\underline{a}}_{\text{phys.}} = -\left(1 + 2\gamma\frac{\phi}{c^2}\right) \tilde{\Pi}^{\perp\,a} + \varepsilon_0(\gamma + 1)\left(\phi^{(0)}_{\text{el.}} \frac{\boldsymbol{\nabla}\phi}{c^2}\right)^{\perp\,a} . \tag{4.5.28}$$

Note that up to the additional second term arising from the additional gravitational coupling in the Lagrangian, this means that the canonical momentum is just minus the displacement (when interpreted as a spatial vector density), as in the non-gravitational case after a PZW transformation.

Now, using the relations in (4.5.27) and (4.5.28), we can express all the interaction terms from (4.5.10d) in terms of 'physical', i.e. tetrad, components of the external electromagnetic quantities. For example, the electric dipole interaction term $\left(1 + (\gamma+1)\frac{\phi(\boldsymbol{R})}{c^2}\right) \frac{\tilde{\mathbf{\Pi}}^\perp(\boldsymbol{R})}{\varepsilon_0} \cdot \boldsymbol{d}$ in the Hamiltonian takes the form

$$\begin{aligned}
&- \left(1 + \frac{\phi(\boldsymbol{R})}{c^2}\right) \sum_a \frac{D^{\perp\,\underline{a}}_{\text{phys.}}(\boldsymbol{R})}{\varepsilon_0} d^{\underline{a}}_{\text{phys.}} + (\gamma+1) \sum_a \left(\phi^{(0)}_{\text{el.}} \frac{\boldsymbol{\nabla}\phi}{c^2}\right)^{\perp\,a}(\boldsymbol{R})\, d^{\underline{a}}_{\text{phys.}} \\
&= -\sqrt{-g_{00}(\boldsymbol{R})} \sum_a \frac{D^{\perp\,\underline{a}}_{\text{phys.}}(\boldsymbol{R})}{\varepsilon_0} d^{\underline{a}}_{\text{phys.}} + (\gamma+1) \sum_a \left(\phi^{(0)}_{\text{el.}} \frac{\boldsymbol{\nabla}\phi}{c^2}\right)^{\perp\,a}(\boldsymbol{R})\, d^{\underline{a}}_{\text{phys.}}
\end{aligned} \tag{4.5.29}$$

when expressed in terms of physical components. The 'gravitational time dilation' factor $\sqrt{-g_{00}}$ in this expression could now also be absorbed by referring the time evolution to the proper time of the observer situated at $\boldsymbol{R}$ instead of coordinate time, leading to a dipole coupling of the usual form '$-\frac{\boldsymbol{D}}{\varepsilon_0} \cdot \boldsymbol{d}$' [Mar95; Läm95] (up to the additional term originating from the additional $\partial_t \boldsymbol{A}^\perp$ coupling in L_{em} (4.4.42)).

Similarly, all the other interaction terms from the Hamiltonian (4.5.10d) can be rewritten in terms of tetrad components. The only difficulty arises when considering the Röntgen term, i.e. the second term in the interaction Hamiltonian, since it involves the momentum $\boldsymbol{P}$, and the similar third term: if the components P_a were just the components of a classical one-form field, there would be no problem in computing its tetrad components as

$$P_{\mathrm{phys.}\underline{a}} = \mathrm{e}_{\underline{a}}^{b}\, P_b = \left(1 - \gamma \frac{\phi(\boldsymbol{R})}{c^2}\right) P_a\,. \tag{4.5.30}$$

However, the P_a are operators that don't commute with the centre of mass position $\boldsymbol{R}$, such that in the application of (4.5.30) one has to deal with with operator ordering ambiguities (which is, of course, a well-known issue regarding curvilinear coordinate transformations in quantum mechanics). Of course, to avoid dealing with these ambiguities, one can stay with the coordinate components of the momentum and rewrite only the *other* quantities in terms of tetrad components, arriving at

$$\frac{1}{2M}\{\boldsymbol{P}\cdot[\boldsymbol{d}\times\boldsymbol{B}(\boldsymbol{R})] + \mathrm{H.c.}\} = \frac{1}{2M}\left\{\sum_a P_a \left(1 - \gamma\frac{\phi(\boldsymbol{R})}{c^2}\right) {}^{(3)}\tilde{\varepsilon}_{\underline{abc}}\, d^{\underline{b}}_{\mathrm{phys.}} B^{\underline{b}}_{\mathrm{phys.}}(\boldsymbol{R}) + \mathrm{H.c.}\right\} \tag{4.5.31}$$

for the Röntgen term, where ${}^{(3)}\tilde{\varepsilon}$ denotes the spatial volume form induced by the physical metric (with tetrad components given by the antisymmetric symbol). When doing so, to give a well-defined geometric meaning to the resulting expression on the right-hand side, one has to keep in mind that the components P_a of the momentum refer to the coordinate basis and the components $d^{\underline{b}}_{\mathrm{phys.}}, B^{\underline{b}}_{\mathrm{phys.}}$ of the dipole moment and the magnetic field refer to the tetrad.

Rewriting all possible terms in the atom–light interaction Hamiltonian in terms of tetrad components, glossing over the just-described ordering ambiguities, we arrive at

$$\begin{aligned} H_{\mathrm{AL,final}} = {} & -\sqrt{-g_{00}(\boldsymbol{R})}\,\frac{\boldsymbol{D}^{\perp}_{\mathrm{phys.}}(\boldsymbol{R})}{\varepsilon_0}\cdot\boldsymbol{d}_{\mathrm{phys.}} + \frac{1}{2M}\{\boldsymbol{P}_{\mathrm{phys.}}\cdot[\boldsymbol{d}_{\mathrm{phys.}}\times\boldsymbol{B}_{\mathrm{phys.}}(\boldsymbol{R})] + \mathrm{H.c.}\} \\ & - \frac{m_1 - m_2}{4m_1m_2}\{\boldsymbol{p}_{\boldsymbol{r}\,\mathrm{phys.}}\cdot[\boldsymbol{d}_{\mathrm{phys.}}\times\boldsymbol{B}_{\mathrm{phys.}}(\boldsymbol{R})] + \mathrm{H.c.}\} \\ & + \frac{1}{8\mu}\left(1 - 2\gamma\frac{\phi(\boldsymbol{R})}{c^2}\right)(\boldsymbol{d}_{\mathrm{phys.}}\times\boldsymbol{B}_{\mathrm{phys.}}(\boldsymbol{R}))^2 + \frac{1}{2\varepsilon_0}\int \mathrm{d}^3\boldsymbol{x}\,\sqrt{-g}\,\boldsymbol{\mathcal{P}}^{\perp\,2}_{d\,\mathrm{phys.}}(\boldsymbol{x},t) \\ & + \int \mathrm{d}^3\boldsymbol{x}\,(\gamma+1)\,\phi^{(0)}_{\mathrm{el.}}\frac{\boldsymbol{\nabla}\phi}{c^2}\cdot\boldsymbol{D}^{\perp}_{\mathrm{phys.}}\,. \end{aligned} \tag{4.5.32}$$

Here we employed 'three-vector' notation also for three-tuples of tetrad components, i.e. a 'dot product' $\boldsymbol{X}_{\mathrm{phys.}}\cdot\boldsymbol{Y}_{\mathrm{phys.}} := \sum_{\underline{a}} X^{\underline{a}}_{\mathrm{phys.}} Y^{\underline{a}}_{\mathrm{phys.}}$ is a scalar product with respect to the *physical* spatial metric, and a 'cross product' $(\boldsymbol{Y}_{\mathrm{phys.}}\times\boldsymbol{Z}_{\mathrm{phys.}})_{\underline{a}} = {}^{(3)}\tilde{\varepsilon}_{\underline{abc}} Y^{\underline{b}}_{\mathrm{phys.}} \boldsymbol{Z}^{\underline{c}}_{\mathrm{phys.}}$ is also defined by the spatial volume form ${}^{(3)}\tilde{\varepsilon}$ induced by the *physical* spatial metric.

To the best of our knowledge, the atom–light interaction terms in the presence of gravity obtained in (4.5.10d) and discussed above are new, save for the electric dipole coupling which was already discussed in [Mar95; Läm95].

Finally, expressing the external field energy (4.5.10e) in terms of tetrad components, i.e. inserting (4.5.27a) and (4.5.28), we obtain

$$\begin{aligned} H_{\mathrm{L,final}} &= \frac{\varepsilon_0}{2} \int \mathrm{d}^3\boldsymbol{x} \left(1 + (1-3\gamma)\frac{\phi}{c^2}\right) \left[(\boldsymbol{D}^{\perp}_{\mathrm{phys.}}/\varepsilon_0)^2 + c^2 \boldsymbol{B}^2_{\mathrm{phys.}}\right] \\ &\quad - \int \mathrm{d}^3\boldsymbol{x}\,(\gamma+1)\,\phi^{(0)}_{\mathrm{el.}} \frac{\boldsymbol{\nabla}\phi}{c^2} \cdot \boldsymbol{D}^{\perp}_{\mathrm{phys.}} \\ &= \frac{\varepsilon_0}{2} \int \mathrm{d}^3\boldsymbol{x}\,\sqrt{-g}\left[(\boldsymbol{D}^{\perp}_{\mathrm{phys.}}/\varepsilon_0)^2 + c^2 \boldsymbol{B}^2_{\mathrm{phys.}}\right] \\ &\quad - \int \mathrm{d}^3\boldsymbol{x}\,(\gamma+1)\,\phi^{(0)}_{\mathrm{el.}} \frac{\boldsymbol{\nabla}\phi}{c^2} \cdot \boldsymbol{D}^{\perp}_{\mathrm{phys.}}\,. \end{aligned} \tag{4.5.33}$$

Up to the second integral, which cancels with the last term from (4.5.32), this is the standard result of the flat-spacetime electromagnetic field energy [Jac98] minimally coupled to gravity [MTW73], as was to be expected.[13]

As we have seen in the previous section for internal energies and in this section for electromagnetic quantities, several terms in the final post-Newtonian Hamiltonian (4.5.10) obtain a natural interpretation when expressed in terms of quantities with direct metric significance, i.e. in terms of components with respect to an orthonormal tetrad frame. Note, however, that such a tetrad (4.5.26) depends on the metric g, i.e. on part of the physical field configuration. This entails that, when comparing physical situations in *different* gravitational fields, i.e. with different physical metrics g, it is not at all conceptually obvious how to relate predictions made for the two situations to each other: even though the *Hamiltonian* looks the same in both cases when expressed in terms of tetrad components, it may be the case that the quantum-mechanical state vector take different forms when expressed in terms of metric quantities in the two situations, due to some specific nature of its preparation procedure (which might, for example, depend on spacetime curvature in some way).

Thus, for a proper interpretation of calculational predictions for experimental situations, one has (in principle) to describe the *whole* experimental situation, including all preparation and measurement procedures, in terms of operationally defined quantities, and express all predicted results in terms of these operational quantities. This is the only way to ensure true coordinate- and frame-independence of predictions.

[13]This result would have been immediate if we did the whole calculation in terms of tetrad components instead of coordinate components, as would have some steps in the calculation of the electromagnetic Lagrangian. However, as stressed in section 4.2.2, the approach based on the background structures with adapted coordinates enabled us to provide a direct comparison with the original calculation of [SB18].

5. Classical perspectives on the Newton–Wigner position observable

This chapter, which is thematically entirely independent from the rest of the thesis, deals with the Newton–Wigner position observable for Poincaré-invariant *classical* systems. To explain at least the little connection to the rest of the thesis that there is, let me (the author) briefly describe how my interest in the topics of this chapter arose. Sonnleitner and Barnett in [SB18], as well as myself in my calculations based on theirs as documented in chapter 4, employed *Newtonian* centre of mass coordinates in the description of a (locally) Poincaré-symmetric composite system, simply for the sake of computational simplicity. This led me to the old question of what kind of central positions one could – or perhaps should? – use for such descriptions. Thus, I was led to extending my knowledge of special-relativistic localisation and position observables, in particular with the beautiful geometric 'hyperplane observable' perspective of Fleming [Fle65]. In the course of this, I wondered if and how one could understand Fleming's 'centre of spin' interpretation of the Newton–Wigner observable in a more geometric way, and also if the quantum Newton–Wigner theorem has a classical analogue (which it 'should' have, morally speaking). This chapter is the outcome of those considerations. We will prove an existence and uniqueness theorem for elementary systems that parallels the well-known Newton–Wigner theorem in the quantum context, and also discuss and justify Fleming's geometric interpretation of the Newton–Wigner position as 'centre of spin'.

Other than in the previous chapters, here we will be fully mathematically rigorous, and also adopt a more mathematical style of presentation. The material in this chapter is also contained in the preprint [SG20], which is under consideration for publication as of the writing of this thesis.

5.1. Introduction

Even though we shall in this chapter exclusively deal with *classical* (i.e. non-quantum) aspects of the Newton–Wigner position observable, we wish to start with a brief discussion of its historic origin, which is based in the early history of relativistic quantum field theory (RQFT). After that we will briefly remark on its classical importance and give an outline of the investigation that is to follow. A more detailed overview of the history of the localisation problem in special-relativistic quantum theory may be found in our preprint [SG20].

As is well-known, the Newtonian concepts of spatial position of elementary, i.e. indecomposable, systems and of centre of mass of composite systems satisfy the expected covariance properties under spatial translations and rotations, and readily translate to ordinary, Galilei-invariant quantum mechanics. There, concepts like 'position operators' and the associated projection operators for positions within any measurable subset of space can be defined, again fulfilling the expected transformation rules under spatial motions.

However, serious difficulties with naive localisation concepts arise in attempts to combine quantum mechanics with special relativity, connected with the fact that negative-energy modes are necessarily introduced if a 'naive position operator' (like multiplying a naive 'wave function' with the position coordinate) is applied to a positive-energy state. However, in 1949, Newton and Wigner showed that it was nevertheless possible to define localised states in a special-relativistic quantum context [NW49]: their method was to write down axioms for what it meant that a system is 'localised in space at a given time' and then investigate existence as well as uniqueness for corresponding position operators. It turned out that existence and uniqueness are indeed given for elementary systems (with fields being elements of irreducible representations of the Poincaré group), except for massless fields of higher helicity. A more rigorous derivation was later given by Wightman [Wig62].

In 1965, Fleming gave a geometric discussion of special-relativistic position observables [Fle65] that highlighted the group-theoretic properties (regarding the group of spacetime automorphisms) underlying several constructions and thereby clarified many of the sometimes controversial issues regarding 'covariance'. Fleming focussed on three position observables which he called 'centre of inertia', 'centre of mass', and the Newton–Wigner position observable, for which he, at the very end of his paper and almost in passing, suggested the name 'centre of spin'. We shall give a more detailed geometric justification for that name in this chapter.

It should be emphasised that the Newton–Wigner notion of localisation still suffers from the acausal spreading of localisation domains that is typical of fields satisfying special-relativistic wave equations, an observation made many times in the literature in one form or another; see, e.g., [SG65; Heg74; Rui81]: if a system is Newton–Wigner localised at a point in space at a time t, it is not strictly localised anymore in any bounded region of space at any time later than t [NW49; WS55]. Conceptual issues of that sort, and related ones concerning, in particular, the relation between Newton–Wigner localisation and the Reeh-Schlieder theorem in RQFT have been discussed many times in the literature even up to the more recent past; see, e.g., [FB99] and [Fle00; Hal01]. For us, however, these quantum field theoretic issues are not the point of interest.

Clearly, due to its historical development, most discussions of Newton–Wigner localisation put their emphasis on its relevance for RQFT: the study of deeply relativistic *classical* systems was simply not considered relevant at the time when special-relativistic localisation was first investigated. However, that has clearly changed with the advent of modern relativistic astrophysics. For example, modern analytical studies of close compact binary-star systems also make use of various definitions of 'centre of mass' in an attempt to separate the 'overall' from the 'internal' motion as far as possible. In that respect, it turns out that modern treatments of gravitationally interacting two-body systems within the theoretical framework of Hamiltonian general relativity show a clear preference for the Newton–Wigner position [Ste11; SJ18], emphasising once more its distinguished role, now in a purely classical context. A concise account of the various definitions of 'centres' that have been used in the context of general relativity is given in [CLS18], which also contains most of the original references in its bibliography. In our opinion, all this provides sufficient motivation for further attempts to work out the characteristic properties of Newton–Wigner localisation in the *classical* realm.

The plan of our investigation is as follows. After setting up our notation and conventions in section 5.2, where we also introduce some mathematical background, we prove a few results in section 5.3 which are intended to explain in what sense the Newton–Wigner position is indeed a 'centre of spin' and in what sense it is uniquely so (theorem 5.3.12). We continue in section 5.4 with the statement and proof of a classical analogue of the Newton–Wigner theorem, according to which the Newton–Wigner position is the unique observable satisfying a set of axioms. The result is presented in theorem 5.4.6 and in a slightly different formulation in theorem 5.4.7. They say that for a classical elementary Poincaré-invariant system with timelike four-momentum (as classified by Arens [Are71a; Are71b]), there is a unique observable transforming 'as a position should' under translations, rotations, and time reversal, having Poisson-commuting components, and satisfying a regularity condition (being C^1 on all of phase space). This observable is the Newton–Wigner position.

5.2. Notation and conventions

This section is meant to list our notation and conventions in the general sense, by also providing some background material on the geometric and group-theoretic setting onto which the following two sections are based.

5.2.1. Minkowski spacetime and the Poincaré group

As before, we use the 'mostly plus' $(-+++)$ signature convention for the spacetime metric and stick to four spacetime dimensions. This is not to say that our analysis cannot be generalised to other dimensions. In fact, as will become clear as we proceed, many of our statements have an obvious generalisation to higher dimensions. On the other hand, as will also become clear, there are a few constructions which would definitely look different in other dimensions, like, e.g., the use of the Pauli–Lubański 'vector' in section 5.2.5, which becomes an $(n-3)$-form in n dimensions, or the classification of elementary systems.

In this chapter, we will view Minkowski spacetime as an affine space M, and the corresponding vector space of 'difference vectors' will be denoted by V. The Minkowski metric will be denoted by $\eta\colon V \times V \to \mathbb{R}$. The isomorphism of V with its dual space V^* induced by η ('index lowering') will be denoted by a superscript 'flat' symbol $\flat$, i.e. for a vector $v \in V$ the corresponding one-form is $v^\flat := \eta(v, \cdot) \in V^*$. The inverse isomorphism ('index raising') will be denoted by a superscript sharp symbol $\sharp$. Note that under a Lorentz transformation Λ, $v \in V$ transforms under the defining representation, $(\Lambda, v) \mapsto \Lambda v$, whereas its image $v^\flat \in V^*$ under the η-induced isomorphism transforms under the inverse transposed, $(\Lambda, v^\flat) \mapsto (\Lambda^{-1})^\top v^\flat = v^\flat \circ \Lambda^{-1}$.

We fix an orientation and a time orientation on M. The (homogeneous) Lorentz group, i.e. the group of linear isometries of (V, η), will be denoted by $\mathcal{L} := \mathrm{O}(V, \eta)$. The Poincaré group, i.e. the group of affine isometries of (M, η), will be denoted by $\mathcal{P}$. The proper orthochronous Lorentz and Poincaré groups (i.e. the connected components of the identity) will be denoted by $\mathcal{L}_+^\uparrow$ and $\mathcal{P}_+^\uparrow$, respectively[1].

We employ standard index notation for Minkowski spacetime, using lowercase Greek letters for spacetime indices. When working with respect to bases, we will, unless otherwise stated, assume them to be positively oriented and orthonormal, and we will use 0 for the timelike and lowercase Latin letters for spatial indices. We will adhere to standard practice in physics where lowering and raising of indices are done while keeping the same kernel symbol; i.e. for a vector $v \in V$ with components v^μ, the components of the corresponding one-form $v^\flat \in V^*$ will be denoted simply by v_μ. For

[1] Note that speaking of just orthochronous or proper Lorentz / Poincaré transformations does not make invariant sense without specifying a time direction.

the sake of notational clarity, we will sometimes denote the Minkowski inner product of two vectors $u, v \in V$ simply by

$$u \cdot v := \eta(u, v) = u_\mu v^\mu. \tag{5.2.1}$$

We fix, once and for all, a reference point / *origin* $o \in M$ in (affine) Minkowski spacetime, allowing us to identify M with its corresponding vector space V (identifying the reference point $o \in M$ with the zero vector $0 \in V$, i.e. via $M \ni x \mapsto (x - o) \in V$), which we will do most of the time. Using the reference point $o \in M$, the Poincaré group splits as a semidirect product

$$\mathcal{P} = \mathcal{L} \ltimes V \tag{5.2.2}$$

where the Lorentz group factor in this decomposition arises as the stabiliser of the reference point – i.e. a Poincaré transformation is considered a homogeneous Lorentz transformation if and only if it leaves o invariant. Thus, a homogeneous Lorentz transformation $\Lambda \in \mathcal{L}$ acts on a point $x \in M \equiv V$ as $(\Lambda x)^\mu = \Lambda^\mu{}_\nu x^\nu$, and a Poincaré transformation $(\Lambda, a) \in \mathcal{P}$ acts as $((\Lambda, a) \cdot x)^\mu = \Lambda^\mu{}_\nu x^\nu + a^\mu$.

We will sometimes make use of the set of spacelike hyperplanes in (affine) Minkowski spacetime M, which we will denote by

$$\mathsf{SpHP} := \{\Sigma \subset M : \Sigma \text{ spacelike hyperplane}\}. \tag{5.2.3}$$

Since the image of a spacelike hyperplane under a Poincaré transformation is again a spacelike hyperplane, there is a natural action of the Poincaré group on SpHP, which we will denote by $((\Lambda, a), \Sigma) \mapsto (\Lambda, a) \cdot \Sigma$ and spell out in more detail in (5.3.4) below.

5.2.2. The Poincaré algebra

When considering the Lie algebra $\mathfrak{p}$ of the Poincaré group (or symplectic representations thereof), we will denote the generators of translations by P_μ such that $a^\mu P_\mu$ is the 'infinitesimal transformation' corresponding to the translation by $a \in V$, and the generators of homogeneous Lorentz transformations (with respect to the chosen origin o) by $J_{\mu\nu}$, such that $-\frac{1}{2}\omega^{\mu\nu} J_{\mu\nu}$ is the 'infinitesimal transformation' corresponding to the Lorentz transformation $\exp(\omega) \in \mathcal{L}_+^\uparrow \subset \mathsf{GL}(V)$ for $\omega \in \mathfrak{l} = \mathrm{Lie}(\mathcal{L}) \subset \mathrm{End}(V)$.

Since we are using the $(-{+}{+}{+})$ signature convention, the minus sign in the expression $-\frac{1}{2}\omega^{\mu\nu} J_{\mu\nu}$ is necessary in order that J_{ab} generate rotations in the e_a–e_b plane from e_a towards e_b, which is the convention we want to adopt. A detailed discussion of these issues regarding sign conventions for the generators of special orthogonal groups can be found in appendix C. Moreover, if $u \in V$ is a future-directed unit timelike vector, then $cP_\mu u^\mu$ (i.e. cP_0 in the Lorentz frame defined by $u = \mathrm{e}_0$), which is *minus* the energy in the frame defined by u, is the generator of active time translations in the direction of u. Therefore, with our conventions, for the case of causal four-momentum $P \in V$ the energy (with respect to future-directed time directions) is positive if and only if P is future-directed.

With our conventions, the commutation relations for the Poincaré generators are as follows:

$$
\begin{aligned}
[P_\mu, P_\nu] &= 0 && (5.2.4a)\\
[J_{\mu\nu}, P_\rho] &= \eta_{\mu\rho} P_\nu - \eta_{\nu\rho} P_\mu && (5.2.4b)\\
[J_{\mu\nu}, J_{\rho\sigma}] &= \eta_{\mu\rho} J_{\nu\sigma} + \text{(antisymm.)} \\
&= \Big(\eta_{\mu\rho} J_{\nu\sigma} - (\mu \leftrightarrow \nu)\Big) - \Big(\rho \leftrightarrow \sigma\Big) && (5.2.4c)
\end{aligned}
$$

As indicated, the abbreviation 'antisymm.' stands for the additional three terms that one obtains by first antisymmetrising (without a factor of $1/2$) in the first pair of indices on the left hand side, here $(\mu\nu)$, and then the ensuing combination once more in the second set of indices, here $(\rho\sigma)$, again without a factor $1/2$.

5.2.3. Symplectic geometry

We employ the following sign conventions for symplectic geometry (as used by Abraham and Marsden in [AM78], but different to those of Arnold in [Arn89]). Let (Γ, ω) be a symplectic manifold. For a smooth function $f \in C^\infty(\Gamma)$, we define the Hamiltonian vector field $X_f \in \mathfrak{X}(\Gamma)$ ($\mathfrak{X}$ denoting the space of smooth vector fields) corresponding to f by

$$\iota_{X_f}\omega := \omega(X_f, \cdot) = \mathrm{d}f, \tag{5.2.5}$$

where ι denotes the interior product between vector fields and differential forms. The Poisson bracket of two smooth functions $f, g \in C^\infty(\Gamma)$ is then defined as

$$\{f, g\} := \omega(X_f, X_g) = \mathrm{d}f(X_g) = \iota_{X_g}\mathrm{d}f. \tag{5.2.6}$$

These conventions give the usual coordinate forms of the Hamiltonian flow equations and the Poisson bracket if the symplectic form ω takes the coordinate form (sign-opposite to that in [Arn89])

$$\omega = \mathrm{d}q^a \wedge \mathrm{d}p_a\,. \tag{5.2.7}$$

It is important to note that $C^\infty(\Gamma)$ as well as $\mathfrak{X}(\Gamma)$ are (infinite dimensional) Lie algebras with respect to the Poisson bracket and the commutator respectively, and that, with respect to these Lie structures, the map $C^\infty(\Gamma) \to \mathfrak{X}(\Gamma), f \mapsto X_f$ is a Lie *anti*-homomorphism, that is,

$$X_{\{f,g\}} = -[X_f, X_g]. \tag{5.2.8}$$

By saying that a one-parameter group $\phi_s\colon \Gamma \to \Gamma$ of symplectomorphisms is *generated* by a function $g \in C^\infty(\Gamma)$, we mean that ϕ_s is the flow of the Hamiltonian vector field to g, i.e. that

$$\frac{\mathrm{d}}{\mathrm{d}s}\phi_s(\gamma) = X_g(\phi_s(\gamma)) \tag{5.2.9}$$

for $\gamma \in \Gamma$, or equivalently

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}s}(f \circ \phi_s) &= \Big(\mathrm{d}f(X_g)\Big) \circ \phi_s \\ &= \{f, g\} \circ \phi_s \end{aligned} \tag{5.2.10}$$

for $f \in C^\infty(\Gamma)$. Here both sides of (5.2.10) are to be understood as evaluated pointwise.

5.2.4. Poincaré-invariant Hamiltonian systems and their momentum maps

A *classical Poincaré-invariant system* will be described by a phase space (Γ, ω) – i.e. a symplectic manifold – with a symplectic action

$$\Phi\colon \mathcal{P} \times \Gamma \to \Gamma,\ ((\Lambda, a), \gamma) \mapsto \Phi_{(\Lambda,a)}(\gamma) \tag{5.2.11}$$

of the Poincaré group (in fact, for most of our purposes an action of $\mathcal{P}_+^\uparrow$ is enough). We will take Φ to be a left action, i.e. to satisfy[2]

$$\Phi_{(\Lambda_1,a_1)} \circ \Phi_{(\Lambda_2,a_2)} = \Phi_{(\Lambda_1\Lambda_2, a_1+\Lambda_1 a_2)}\,. \tag{5.2.12}$$

We will denote such systems as (Γ, ω, Φ).

The left action Φ of $\mathcal{P}$ on Γ induces vector fields V_ξ on Γ (the so-called *fundamental vector fields*), one for each ξ in the Lie algebra $\mathfrak{p}$ of $\mathcal{P}$. They are given by

$$V_\xi(\gamma) := \frac{\mathrm{d}}{\mathrm{d}s}\Phi_{\exp(s\xi)}(\gamma)\bigg|_{s=0}\,, \tag{5.2.13}$$

so that the map $\mathfrak{p} \to \mathfrak{X}(\Gamma), \xi \mapsto V_\xi$, given by the differential of Φ with respect to its first argument and evaluated at the group identity, is clearly linear. In fact, it is

[2] We refer to [Giu15] for a detailed discussion of left versus right actions and the corresponding sign conventions that will also play an important role in the following.

straightforward to show that it is an anti-homomorphism from the Lie algebra $\mathfrak{p}$ into the Lie algebra $\mathfrak{X}(M)$,[3] i.e.

$$[V_{\xi_1}, V_{\xi_2}] = -V_{[\xi_1,\xi_2]}. \tag{5.2.14}$$

Moreover, a similar calculation shows [Giu15, appendix B]

$$(\mathrm{D}\Phi_{(\Lambda,a)}) \circ V_\xi = V_{\mathrm{Ad}_{(\Lambda,a)}(\xi)} \circ \Phi_{(\Lambda,a)} , \tag{5.2.15}$$

where $\mathrm{D}\Phi_{(\Lambda,a)} \colon T\Gamma \to T\Gamma$ denotes the differential of $\Phi_{(\Lambda,a)} \colon \Gamma \to \Gamma$.

As $\mathcal{P}$ acts by symplectomorphisms, the fundamental vector fields V_ξ are locally Hamiltonian, i.e. locally (in a neighbourhood of each point), for each $\xi \in \mathfrak{p}$ there exists a local function f_ξ such that $\mathrm{d}f_\xi = \iota_{V_\xi}\omega$. In fact, due to the Poincaré algebra being perfect (in spacetime dimension greater than 2), the f_ξ can be shown to exist globally, so that each V_ξ is a globally defined Hamiltonian vector field (i.e. each one-parameter group $\Phi_{\exp(s\xi)} \colon \Gamma \to \Gamma$ of symplectomorphisms is generated, in the sense of (5.2.10), by the corresponding function f_ξ). Moreover, due to $\mathfrak{p}$ having vanishing second cohomology, the f_ξ can be chosen in such a way that the map $\xi \mapsto f_\xi$ from the Lie algebra $\mathfrak{p}$ to the Lie algebra $C^\infty(\Gamma)$ (the Lie product of the latter being the Poisson bracket) is a Lie homomorphism, i.e.

$$\{f_{\xi_1}, f_{\xi_2}\} = f_{[\xi_1,\xi_2]}. \tag{5.2.16}$$

I.e., for spacetime dimension greater than 2, any symplectic action of the Poincaré group is always a *Poisson action*. Details of these arguments may be found in [SG20]. Note that, according to (5.2.14) and (5.2.8), both maps $\xi \mapsto V_\xi$ and $V_\xi \mapsto f_\xi$ are Lie *anti*-homomorphisms. Hence their combination $\xi \mapsto f_\xi$ is a proper Lie homomorphism (no minus sign on the right-hand side of (5.2.16)).

Now, we will deduce the transformation properties of the generators f_ξ under the action of $\mathcal{P}$. Taking the pullback of the equation $\omega(V_\xi, \cdot) = \mathrm{d}f_\xi$ with $\Phi_{(\Lambda,a)^{-1}}$ and using the invariance of ω as well as (5.2.15), we immediately deduce

$$\Phi^*_{(\Lambda,a)^{-1}} f_\xi := f_\xi \circ \Phi_{(\Lambda,a)^{-1}} = f_{\mathrm{Ad}_{(\Lambda,a)}(\xi)} , \tag{5.2.17}$$

which may also be read as the invariance of the real-valued function $f \colon \mathfrak{p} \times \Gamma \to \mathbb{R}$, $(\xi, \gamma) \mapsto f_\xi(\gamma)$, under the combined left action of $\mathcal{P}$ on $\mathfrak{p} \times \Gamma$ given by $\mathrm{Ad} \times \Phi$. Alternatively, since $\xi \mapsto f_\xi$ is linear, we may regard f as $\mathfrak{p}^*$-valued function on Γ, where $\mathfrak{p}^*$ denotes the vector space dual to $\mathfrak{p}$. This map is called the *momentum map*[4] for the given system (Γ, ω, Φ), which according to (5.2.17) is then Ad^*-equivariant:

$$f \circ \Phi_{(\Lambda,a)} = \mathrm{Ad}^*_{(\Lambda,a)} \circ f \iff \mathrm{Ad}^*_{(\Lambda,a)} \circ f \circ \Phi_{(\Lambda,a)^{-1}} = f \tag{5.2.18}$$

[3] Had we chosen Φ to be a right action, we would have obtained a proper Lie homomorphism; compare [Giu15, appendix B].

[4] See [AM78, chap. 4.2] for a general discussion on the notion of 'momentum map' and also [Giu15] for an account of its use and properties restricted to the case of Poincaré-invariant systems.

The second expression is again meant to stress that the condition of equivariance is equivalent to the invariance of the function f under the combined left actions in its domain and target spaces (invariance of the graph). Note that Ad^* denotes the co-adjoint representation of $\mathcal{P}$ on $\mathfrak{p}^*$, given by $\mathrm{Ad}^*_{(\Lambda,a)} := (\mathrm{Ad}_{(\Lambda,a)^{-1}})^\top$ with superscript $\top$ denoting the transposed map.

Points in Γ faithfully represent the state of the physical system whereas observables correspond to functions on Γ. In order to implement time evolution we shall employ a 'classical Heisenberg picture', in which the phase space point remains the same at all times, whereas the evolution will correspond to the changes of observables according to their association to different spacelike hyperplanes in spacetime. Although this is different from the ('Schrödinger picture') approach usually taken in classical mechanics (where the state of the system is given by a phase space point changing in 'time', which is an external parameter), this point of view is clearly better adapted to the Poincaré-relativistic framework, in which there simply is no absolute notion of time.

Choosing a set of ten basis vectors $(P_\mu, J_{\mu\nu})$ for $\mathfrak{p}$ obeying (5.2.4) (compare appendix C), we can contract the $\mathfrak{p}^*$-valued momentum map with each of these basis vectors in order to obtain the corresponding ten real-valued component functions of the momentum map. By some abuse of notation we shall call these component functions by the same letters $(P_\mu, J_{\mu\nu})$ as the Lie algebra elements themselves. (5.2.16) now says that the map that sends the Lie algebra elements P_μ and $J_{\mu\nu}$ in $\mathfrak{p}$ to the corresponding component functions of the momentum map is a Lie homomorphism from $\mathfrak{p}$ to the Lie algebra $C^\infty(\Gamma, \mathbb{R})$ (the latter with Poisson bracket as Lie multiplication):

$$\{P_\mu, P_\nu\} = 0 \tag{5.2.19a}$$

$$\{J_{\mu\nu}, P_\rho\} = \eta_{\mu\rho} P_\nu - \eta_{\nu\rho} P_\mu \tag{5.2.19b}$$

$$\{J_{\mu\nu}, J_{\rho\sigma}\} = \eta_{\mu\rho} J_{\nu\sigma} + \text{(antisymm.)} \tag{5.2.19c}$$

The Ad^*-equivariance of the momentum map can now be written down in component form if we first set $\xi = P_\mu$ and then $\xi = J_{\mu\nu}$. Indeed, considering (5.2.17) and recalling our abuse of notation in denoting the real-valued phase space functions f_{P_μ} and $f_{J_{\mu\nu}}$ again with the letters P_μ and $J_{\mu\nu}$, we can immediately read from (D.8) of appendix D, in which we need to replace e_a with P_μ and B_{ab} with $-J_{\mu\nu}$ according to (C.13) of appendix C, that

$$P_\mu \circ \Phi_{(\Lambda,a)} = (\Lambda^{-1})^\nu{}_\mu \, P_\nu \,, \tag{5.2.20a}$$

$$J_{\mu\nu} \circ \Phi_{(\Lambda,a)} = (\Lambda^{-1})^\rho{}_\mu (\Lambda^{-1})^\sigma{}_\nu \, J_{\rho\sigma} + a_\mu (\Lambda^{-1})^\rho{}_\nu \, P_\rho - a_\nu (\Lambda^{-1})^\rho{}_\mu \, P_\rho \,. \tag{5.2.20b}$$

Note that the left-hand sides of (5.2.20) are precisely what we need; that is, we need the composition with $\Phi_{(\Lambda,a)}$ rather than $\Phi_{(\Lambda,a)^{-1}}$ to evaluate the momenta P_μ and $J_{\mu\nu}$ on the actively Poincaré-displaced phase space points. Note also that if we had put the indices upstairs and had used, e.g., $P^\mu = \eta^{\mu\nu} P_\nu$ rather than P_μ then the right-hand side of (5.2.20a) would read $\Lambda^{\mu}{}_{\nu} P^{\nu}$, and correspondingly in (5.2.20b). Finally recall that the last term on the right-hand side of (5.2.20b) just reflects the familiar transformation of angular momentum (the momentum associated to spatial rotations) under spatial translations, which is typical for the *co*-adjoint representation, which here gets extended to the momentum associated to boost transformations[5].

5.2.5. The Pauli–Lubański vector

Given a classical Poincaré-invariant system, the Pauli–Lubański vector W is the V-valued phase space function defined in components by

$$W_\mu = -\frac{1}{2}\varepsilon_{\mu\nu\rho\sigma}P^\nu J^{\rho\sigma} \tag{5.2.21}$$

where ε denotes the volume form of Minkowski space (whose components in a positively oriented orthonormal basis are just given by the usual totally antisymmetric symbol, with $\varepsilon_{0123} = +1$). The sign convention in this definition can be understood as follows. We imagine a situation in which P is timelike and future-directed (positive energy, see above), and consider the spatial components of W with respect to an orthonormal basis $\{\mathrm{e}_0, \dots, \mathrm{e}_3\}$ of V with $(\mathrm{e}_0)^\mu = P^\mu / \sqrt{-P_\nu P^\nu}$ ('momentum rest frame'). For those, we obtain

$$\frac{W_a}{\sqrt{-P_\mu P^\mu}} = -\frac{1}{2}\varepsilon_{a0\rho\sigma}J^{\rho\sigma} = \frac{1}{2}{}^{(3)}\varepsilon_{abc}J^{bc} \tag{5.2.22}$$

where the ${}^{(3)}\varepsilon_{abc}$ is the three-dimensional antisymmetric symbol / the components of the spatial volume form. Thus, since $J^{bc} = J_{bc}$ generates rotations from e_b towards e_c, we see that $W_a / \sqrt{-P_\mu P^\mu}$ generates rotations 'along the e_a axis' in the usual, three-dimensional sense. Thus, $W / \sqrt{-P_\mu P^\mu}$ can be interpreted as the 'spatial spin vector' in the momentum rest frame, which is the usual interpretation of the Pauli–Lubański vector.

Rewriting the definition of W as

$$W_\mu = -\frac{1}{2}\varepsilon_{\mu\nu\rho\sigma}P^\nu J^{\rho\sigma} = \frac{1}{2}\varepsilon_{\nu\rho\sigma\mu}P^\nu J^{\rho\sigma} = \frac{1}{3!}\varepsilon_{\nu\rho\sigma\mu}(P^\flat \wedge J)^{\nu\rho\sigma}, \tag{5.2.23}$$

we see that in the language of exterior algebra

$$W = (*(P^\flat \wedge J))^\sharp \tag{5.2.24}$$

where $*$ is the Hodge star operator. Here we use the standard sign conventions for the Hodge operator, i.e. the definition $\alpha \wedge *\beta = \eta(\alpha, \beta)\, \varepsilon$; see for example [Str13] or [Giu15, appendix A].

[5]One easily checks that the signs are right: translating a system whose momentum points in y-direction by a positive amount into the x-direction should enhance the angular momentum in z-direction. This is just what (5.2.20b) implies.

5.3. The Newton–Wigner position as a 'centre of spin'

In this section we will explain our understanding and present our geometric clarification of Fleming's statement in [Fle65] that the Newton–Wigner position may be understood as a 'centre of spin'. To this end, we introduce Fleming's geometric framework for special-relativistic position observables, and then discuss the definition of position observables by spin supplementary conditions (SSCs). Finally, we introduce the notion of a position observable being a 'centre of spin', and prove that the Newton–Wigner position is the only continuous position observable defined by an SSC that represents a centre of spin in that sense.

5.3.1. Position observables on spacelike hyperplanes

We start by describing the general framework developed by Fleming in [Fle65] and also [Fle66] for the description of special-relativistic position observables, translated to our case of classical systems from Fleming's quantum language. Consider a classical Poincaré-invariant system (Γ, ω, Φ). By a *position observable* χ for this system we understand a 'procedure' which, given any spacelike hyperplane $\Sigma \in \mathrm{SpHP}$ in (affine) Minkowski spacetime, allows us to 'localise' the system on Σ. More precisely, this means that for any $\Sigma \in \mathrm{SpHP}$, we have an M-valued phase space function

$$\chi(\Sigma) \colon \Gamma \to M \tag{5.3.1}$$

with image contained in Σ, whose value $\chi(\Sigma)(\gamma)$ for $\gamma \in \Gamma$ is to be interpreted as the 'χ-position' of our system in state γ on the hyperplane Σ.

Any spacelike hyperplane $\Sigma \in \mathrm{SpHP}$ is uniquely characterised by its (timelike) future-directed unit normal $u \in V$ and its distance $\tau \in \mathbb{R}$ to the origin $o \in M$, measured along the straight line through o in direction u. In terms of these, it has the form

$$\Sigma = \{x \in M : u_\mu x^\mu = -\tau\}, \tag{5.3.2}$$

where we identified M with V. From now on, whenever convenient, we will identify Σ with the tuple (u, τ). The condition that the image of $\chi(\Sigma)$ be contained in Σ then takes the form

$$u_\mu \chi^\mu(u, \tau)(\gamma) = -\tau. \tag{5.3.3}$$

We can now also spell out explicitly the left action of $\mathcal{P}$ on SpHP that is induced from the left action of $\mathcal{P}$ on M (as already mentioned below (5.2.3)):

$$(\Lambda, a) \cdot (u, \tau) = (\Lambda u, \tau - \Lambda u \cdot a) \tag{5.3.4}$$

Fixing u and varying τ in (5.3.2), we obtain the spacelike hyperplanes corresponding to different 'instants of time' τ in the Lorentz frame corresponding to u. Thus, for a fixed state $\gamma \in \Gamma$ and fixed frame u, the set

$$\{\chi(u,\tau)(\gamma) : \tau \in \mathbb{R}\} \subset M \tag{5.3.5}$$

gives the 'worldline' of the χ-position of the system. Following Fleming [Fle65], who says that this is a requirement 'easily agreed upon', we require that this worldline should be parallel to the four-momentum[6], i.e. $\frac{\partial \chi(u,\tau)}{\partial \tau} \propto P$. Together with (5.3.3), this implies condition (5.3.8) in the definition below, which is meant to sum up all the preceding considerations.

Definition 5.3.1. A *position observable* for a classical Poincaré-invariant system (Γ, ω, Φ) with causal four-momentum is a map

$$\chi \colon \mathsf{SpHP} \times \Gamma \to M, \; (\Sigma, \gamma) \mapsto \chi(\Sigma)(\gamma) \tag{5.3.6}$$

satisfying

$$\chi(\Sigma)(\gamma) \in \Sigma \tag{5.3.7}$$

for all $\Sigma \in \mathsf{SpHP}$ and all $\gamma \in \Gamma$ (or, equivalently, (5.3.3)), as well as

$$\frac{\partial \chi_\mu(u,\tau)}{\partial \tau} = \frac{1}{(-u \cdot P)} P_\mu \,. \tag{5.3.8}$$

For fixed $\Sigma \in \mathsf{SpHP}$, we will often view $\chi(\Sigma) \colon \Gamma \to M$ as a phase space function in its own right.

Note that (5.3.8) and (5.3.3) imply that the four-momentum must be causal for such a position observable to exist.

In addition to the demands of the positions $\chi(\Sigma)$ being located on Σ and of 'worldlines' in direction of the four-momentum, Fleming also introduces the following covariance requirement (which we, different to Fleming, do not include in the definition of a position observable):

Definition 5.3.2. A position observable for a classical Poincaré-invariant system (Γ, ω, Φ) is said to be *covariant* if and only if

$$\chi\Big((\Lambda, a) \cdot \Sigma\Big)\Big(\Phi_{(\Lambda,a)}(\gamma)\Big) = (\Lambda, a) \cdot \Big(\chi(\Sigma)(\gamma)\Big) \tag{5.3.9}$$

for all $\Sigma \in \mathsf{SpHP}$, $\gamma \in \Gamma$ and $(\Lambda, a) \in \mathcal{P}$. This can be read concisely as saying that the map (5.3.6) is invariant under the natural left action induced from those on the domain and target spaces (invariance of χ's graph):

$$\chi = (\Lambda, a) \circ \chi \circ \Big((\Lambda, a)^{-1} \times \Phi_{(\Lambda,a)^{-1}}\Big) \,. \tag{5.3.10}$$

[6]This assumption is natural for closed systems as we consider here. For non-closed systems, i.e. systems without local energy–momentum conservation, the four-velocity is in general not parallel to the four-momentum; see, e.g., the discussion at the beginning of section 2.6 in [Giu18].

This is indeed a sensible notion of covariance: it demands that, for any Poincaré transformation (Λ, a), the χ-position of the transformed system $\Phi_{(\Lambda,a)}(\gamma)$ on the transformed hyperplane $(\Lambda, a) \cdot \Sigma$ be the transform of the 'original position' $\chi(\Sigma)(\gamma)$. In terms of components, (5.3.9) assumes the form

$$\chi^\mu(\Lambda u, \tau - \Lambda u \cdot a) \circ \Phi_{(\Lambda,a)} = \Lambda^\mu{}_\nu \chi^\nu(u, \tau) + a^\mu \,, \tag{5.3.11}$$

taking into account (5.3.4).

5.3.2. Spin supplementary conditions

The most important and widely used procedure to define special-relativistic position observables is by so-called *spin supplementary conditions*. Suppose we are given a causal, future-directed vector $P \in V$ and an antisymmetric 2-tensor $J \in \bigwedge^2 V^*$, describing the four-momentum and the angular momentum (with respect to the origin $o \in M$) of some physical system. For any future-directed timelike vector $f \in V$, we then consider the equation

$$0 = S_{\mu\nu} f^\nu \tag{5.3.12}$$

with $S_{\mu\nu} := J_{\mu\nu} - x_\mu P_\nu + x_\nu P_\mu$, which we view as an equation for $x \in M$. Since S is the angular momentum tensor with respect to the reference point x (instead of the origin o as for J), or the *spin tensor* with respect to x, (5.3.12) is called the *spin supplementary condition* (SSC) with respect to f. As is well-known (and easily verified), the set of its solutions x is a line in M with tangent P, namely

$$\{x \in M : 0 = S_{\mu\nu} f^\nu\} = \left\{ x \in M : x_\mu = \frac{J_{\mu\rho} f^\rho}{f \cdot P} + \lambda P_\mu \text{ with } \lambda \in \mathbb{R} \right\}. \tag{5.3.13}$$

This line can be given the interpretation of the 'centre of energy' worldline of our system with respect to the Lorentz frame defined by f. See [CLS18] and references therein for further discussion on the interpretation and impact of various SSCs as regards equations of motion in general relativity.

The idea is now to explicitly combine the SSC-based approach with Fleming's geometric ideas, thereby introducing the two independent parameters f from (5.3.13) and u from (5.3.2). We define a position observable in the sense of definition 5.3.1 in the following way: given a classical Poincaré-invariant system (Γ, ω, Φ) with causal four-momentum and a state $\gamma \in \Gamma$, we consider the SSC worldline defined by (5.3.12) where we now take $P_\mu(\gamma)$ for the four-momentum and $J_{\mu\nu}(\gamma)$ for the angular momentum tensor. We then simply define $\chi(\Sigma)(\gamma)$ to be the intersection of this worldline with the hyperplane $\Sigma = (u, \tau)$. This means that we take the $x(\lambda)$ from (5.3.13) and determine the parameter λ from (5.3.3), i.e. from $x(\lambda) \cdot u + \tau = 0$. Inserting the $\lambda = \lambda(u, \tau)$ so determined leads to

Definition 5.3.3. The SSC *position observable* with respect to f is given by

$$\chi_\mu(u,\tau) = \frac{J_{\mu\rho} f^\rho}{f \cdot P} + \frac{\tau P_\mu}{(-u \cdot P)} - \frac{J_{\lambda\rho} u^\lambda f^\rho}{(-f \cdot P)} \frac{P_\mu}{(-u \cdot P)} \,. \tag{5.3.14}$$

Let us again stress the interpretation of this expression: it is the SSC position with respect to f (i.e. a point on the 'centre of energy' worldline with respect to f) as localised on the hyperplane characterised by unit normal u and distance τ to the origin, i.e. as seen in the Lorentz frame with respect to u at 'time' τ.

Note that for this definition to make sense, f does not have to be a fixed timelike future-directed vector: it can depend on the normal u (and could even depend on τ), and it can also depend on phase space[7]. Of course this means that according to this dependence of f, we will possibly be considering different worldlines for different choices of u.

Example 5.3.4. (i) Choosing $f = u$, we are considering, for each u, the SSC worldline with respect to u, i.e. the *centre of energy* worldline[8] with respect to u. Using (5.3.14), the centre of energy position observable has the form

$$\chi_\mu^{\mathrm{CE}}(u,\tau) = \frac{J_{\mu\rho} u^\rho}{u \cdot P} + \frac{\tau P_\mu}{(-u \cdot P)} \,. \tag{5.3.15}$$

(ii) In the case of timelike four-momentum, we can choose $f = P$ the four-momentum (the Tulczyjew–Dixon SSC), such that the corresponding SSC worldline is the centre of energy worldline in the momentum rest frame of the system. This worldline, which is obviously independent of u, was called the *centre of inertia* worldline by Fleming [Fle65]. The centre of inertia has the form

$$\chi_\mu^{\mathrm{CI}}(u,\tau) = -\frac{J_{\mu\rho} P^\rho}{m^2 c^2} + \frac{\tau P_\mu}{(-u \cdot P)} - \frac{J_{\lambda\rho} u^\lambda P^\rho}{m^2 c^2} \frac{P_\mu}{(-u \cdot P)} \,, \tag{5.3.16}$$

where $m = \sqrt{-P^2}/c$ is the mass of the system.

[7] Various choices for f were given distinguished names in the literature. The main ones, different from the Newton–Wigner condition to be discussed here, are as follows. If f is meant to just characterise a fixed 'laboratory frame', which may be preferred for any reason, like rotational symmetries in that frame, the SSC is named after Corinaldesi & Papapetrou [CP51]. If f is proportional to the total linear momentum of the system, the SSC is named after Tulczyjew [Tul59] and Dixon [Dix70]. If f is chosen in a somewhat self-referential way to be the four-velocity of the worldline that is to be determined by the very SSC containing that f, the condition is named after Frenkel [Fre26], Mathisson [Mat37; Mat10], and Pirani [Pir56; Pir09].

[8] Note that it was called 'centre of mass' by Fleming [Fle65].

(iii) Choosing $f = u + \frac{P}{mc}$ where $m = \sqrt{-P^2}/c$ is the mass of the system (again only possible in the case of timelike four-momentum), we obtain the *Newton–Wigner position observable*. Evaluating (5.3.14), it has the form

$$\chi^{\mathrm{NW}}_\mu(u,\tau) = -\frac{J_{\mu\rho}\left(u^\rho + \frac{P^\rho}{mc}\right)}{mc - u\cdot P} + \frac{\tau P_\mu}{(-u\cdot P)} - \frac{J_{\lambda\rho}u^\lambda P^\rho}{mc(mc - u\cdot P)}\,\frac{P_\mu}{(-u\cdot P)}\,. \tag{5.3.17}$$

Of course, the SSC position observable (5.3.14) will generally not be covariant in the sense of definition 5.3.2 unless f is also assumed to transform appropriately. If f depends on $\Sigma \in \mathsf{SpHP}$ and $\gamma \in \Gamma$ and takes values in V it seems obvious that for the resulting position to be covariant f itself must be a covariant function under the combined actions on its domain and target spaces. Indeed, we have

Proposition 5.3.5. *If the vector f defining the SSC position observable χ is a function*

$$f\colon \mathsf{SpHP}\times\Gamma \to V, \quad (\Sigma,\gamma)\mapsto f(\Sigma)(\gamma), \tag{5.3.18}$$

such that

$$f\Big((\Lambda,a)\cdot\Sigma\Big)\Big(\Phi_{(\Lambda,a)}(\gamma)\Big) = \Lambda\cdot\Big(f(\Sigma)(\gamma)\Big) \tag{5.3.19}$$

for all $\Sigma \in \mathsf{SpHP}$, $\gamma\in\Gamma$, and $(\Lambda,a)\in\mathcal{P}$, then χ is a covariant position observable. Again we note that, just like in the transition from (5.3.9) *to* (5.3.10)*, we may rewrite* (5.3.19) *equivalently as expressing the invariance of f (i.e. its graph) under simultaneous actions on its domain and target spaces (using that translations act trivially on the target space V):*

$$f = \Lambda\circ f\circ\Big((\Lambda,a)^{-1}\times\Phi_{(\Lambda,a)^{-1}}\Big) \tag{5.3.20}$$

Proof. At first, suppose we are given a future-directed timelike four-momentum $P\in V$ and an angular momentum tensor $J\in\bigwedge^2 V^*$, as well as a future-directed timelike vector f for the definition of an SSC. In addition, fix a Poincaré transformation $(\Lambda,a)\in\mathcal{P}$. If we now consider (a) the SSC worldline for P and J with respect to f, and (b) the SSC worldline for the transformed four-momentum $P' = \Lambda P$ and angular momentum $J' = ((\Lambda^{-1})^\top\otimes(\Lambda^{-1})^\top)J + a^\flat\wedge(\Lambda^{-1})^\top P^\flat$ (compare (5.2.20b)) with respect to the transformed vector Λf, it is easy to check that the second worldline is the Poincaré transform by (Λ,a) of the first. That is, by Poincaré transforming the four-momentum and angular momentum of the system as well as the 'direction vector' for the SSC, we Poincaré transform the SSC worldline.

Now, the SSC position $\chi(\Sigma)(\gamma)$ is defined to be the intersection of the hyperplane Σ with the SSC worldline of γ with respect to $f(\Sigma)(\gamma)$. Thus, the 'new position'

$$\chi\Big((\Lambda,a)\cdot\Sigma\Big)\Big(\Phi_{(\Lambda,a)}(\gamma)\Big) \tag{5.3.21}$$

is the intersection of the transformed hyperplane $(\Lambda, a) \cdot \Sigma$ with the SSC worldline of the transformed system $\Phi_{(\Lambda,a)}(\gamma)$ with respect to the transformed vector $\Lambda \cdot \Big(f(\Sigma)(\gamma)\Big)$, where we used the covariance requirement (5.3.19). But according to our earlier considerations, this means that the 'new position' is the intersection of the transformed hyperplane with the transform of the original SSC worldline – i.e. the transform of the original position $\chi(\Sigma)(\gamma)$. This means that the position observable is covariant. $\square$

Since the vectors defining the centre of energy, the centre of inertia and the Newton–Wigner position satisfy (5.3.19), all of these are covariant position observables. We stress once more that for this to be true we need to take into account the action of the Poincaré group on SpHP. This remark is particularly relevant in the Newton–Wigner case, in which f is the sum of two vectors, u and $P/(mc)$, the first being associated to an element of SpHP and the second to an element of Γ. Covariance cannot be expected to hold for non-trivial actions on Γ alone. In the next section we will offer an insight as to why this somewhat 'hybrid' combination for f in terms of an 'external' vector u and an 'internal' vector $P/(mc)$ appears. The latter is internal, or dynamical, in the sense that it is defined entirely by the physical state of the system, i.e. a point in Γ, while the former is external, or kinematical, in the sense that it refers to the choice of $\Sigma \in$ SpHP, which is entirely independent of the physical system and its state.

Finally, we will need the following well-known result for SSCs with respect to different vectors f, which was first shown by Møller in 1949 in [Møl49]; see also [Giu15, theorem 17] for a recent and more geometric discussion:

Theorem 5.3.6 (Møller disc and radius)**.** *Suppose we are given the future-directed timelike four-momentum vector $P \in V$ and the angular momentum tensor $J \in \bigwedge^2 V^*$ of some physical system. Consider the bundle of all possible SSC worldlines* (5.3.13) *for this system, defined by considering all future-directed timelike vectors f. The intersection of this bundle with any hyperplane $\Sigma \in$* SpHP *orthogonal to P is a two-dimensional disc (the so-called* Møller disc*) in the plane orthogonal to the Pauli–Lubański vector $W = (*(P^\flat \wedge J))^\sharp$, whose centre is the centre of inertia on Σ and whose radius is the* Møller radius

$$R_M = \frac{S}{mc}\,, \tag{5.3.22}$$

where $S = \sqrt{W^2}/(mc)$ is the spin of the system and $m = \sqrt{-P^2}/c$ its mass.

5.3.3. The centre of spin condition

For a system with timelike four-momentum, the Pauli–Lubański vector W has the interpretation of being (mc times) the spin vector in the momentum rest frame. We now define the spin vector in an arbitrary Lorentz frame by boosting $W/(mc)$ to the new frame:

Definition 5.3.7. Given the timelike four-momentum $P \in V$ and the Pauli–Lubański vector $W \in P^\perp$ of a physical system, its *spin vector* in the Lorentz frame given by the future-directed unit timelike vector u is

$$s(u) := B(u) \cdot \frac{W}{mc}\,, \tag{5.3.23}$$

where $B(u) \in \mathcal{L}_+^\uparrow$ is the unique Lorentz boost with respect to $\frac{P}{mc}$ (i.e. containing $\frac{P}{mc}$ in its timelike 2-plane of action) that maps $\frac{P}{mc}$ to u, with $m = \sqrt{-P^2}/c$ being the mass. In terms of components, this boost is given by[9]

$$B^\mu{}_\nu(u) = \delta^\mu_\nu + \frac{\left(\frac{P^\mu}{mc} + u^\mu\right)\left(\frac{P_\nu}{mc} + u_\nu\right)}{1 - u \cdot \frac{P}{mc}} - 2\frac{u^\mu P_\nu}{mc}\,. \tag{5.3.24}$$

Definition 5.3.8. A *centre of spin* position observable for a classical Poincaré-invariant system (Γ, ω, Φ) with timelike four-momentum is a position observable χ satisfying

$$s_\mu(u) = -\frac{1}{2}\varepsilon_{\mu\nu\rho\sigma} u^\nu S^{\rho\sigma}(u), \tag{5.3.25}$$

where $S_{\rho\sigma}(u) := J_{\mu\nu} - \chi_\mu(u,\tau)P_\nu + \chi_\nu(u,\tau)P_\mu$ is the spin tensor[10] with respect to χ. Expressed in terms of the Hodge operator, this condition reads

$$s(u) = (*(u^\flat \wedge S(u)))^\sharp. \tag{5.3.26}$$

With respect to an orthonormal basis $\{u = \mathrm{e}_0, \ldots, \mathrm{e}_3\}$ adapted to u, the centre of spin condition takes the form

$$s_0(u) = 0, \quad s_a(u) = -\frac{1}{2}\varepsilon_{a0\rho\sigma} S^{\rho\sigma}(u) = \frac{1}{2}{}^{(3)}\varepsilon_{abc} S^{bc}(u), \tag{5.3.27}$$

through which it acquires an immediate interpretation: a position observable is a centre of spin if and only if, for any Lorentz frame u, the spin vector defined by boosting the Pauli–Lubański vector to u really generates spatial rotations around the point given by the position observable.

[9] Generally, given two unit timelike future-pointing vectors n_1 and n_2, then the boost that maps n_1 onto n_2 and fixes the spacelike plane orthogonal to $\mathrm{span}\{n_1, n_2\}$ is given by the combination $\rho_{n_1+n_2} \circ \rho_{n_1}$ of two hyperplane-reflections, where $\rho_n := \mathrm{id}_V - 2\frac{n \otimes n^\flat}{n^2}$ is the reflection at the hyperplane orthogonal to n. Setting $n_1 = P/(mc)$ and $n_2 = u$ gives (5.3.24).

[10] Since $\frac{\partial \chi(u,\tau)}{\partial \tau}$ is proportional to P, the spin tensor is independent of τ.

We will now rewrite the centre of spin condition. Since $S(u) = J - (\chi(u,\tau))^\flat \wedge P^\flat$, we can rewrite the Pauli–Lubański vector as $W = \left[* \left(\frac{P^\flat}{mc} \wedge J \right) \right]^\sharp = \left[* \left(\frac{P^\flat}{mc} \wedge S(u) \right) \right]^\sharp$. Thus, the centre of spin condition takes the form

$$(B(u)^{-1})^\top \left[* \left(\frac{P^\flat}{mc} \wedge S(u) \right) \right] = *(u^\flat \wedge S(u)). \tag{5.3.28}$$

Since $B(u)$ is a Lorentz transformation, i.e. an isometry of (V, η), and it maps $P/(mc)$ to u, this is equivalent to

$$u^\flat \wedge \left((B(u)^{-1})^\top \otimes (B(u)^{-1})^\top \right) (S(u)) = u^\flat \wedge S(u). \tag{5.3.29}$$

Using the explicit form (5.3.24) of $B(u)$, we see that

$$\left((B(u)^{-1})^\top \otimes (B(u)^{-1})^\top \right) (S(u)) = S(u) + \frac{\frac{P^\flat}{mc} \wedge \left(\iota_{u + \frac{P}{mc}} S(u) \right)}{1 - u \cdot \frac{P}{mc}} + u^\flat \wedge (\ldots). \tag{5.3.30}$$

Thus, we have the following:

Lemma 5.3.9. *The centre of spin condition is equivalent to*

$$u^\flat \wedge P^\flat \wedge \left(\iota_{u + \frac{P}{mc}} S(u) \right) = 0. \tag{5.3.31}$$

□

Since the Newton–Wigner position observable is defined by the SSC $\iota_{u + \frac{P}{mc}} S(u) = 0$, the preceding result immediately implies

Theorem 5.3.10. *The Newton–Wigner position observable χ^{NW} is a centre of spin.* □

Further rewriting the centre of spin condition, we see that (5.3.31) is equivalent to

$$\iota_{u + \frac{P}{mc}} S(u) \in \operatorname{span}\{u^\flat, P^\flat\}. \tag{5.3.32}$$

Due to the antisymmetry of $S(u)$, this is equivalent to

$$\iota_{u + \frac{P}{mc}} S(u) \in \operatorname{span} \left\{ u^\flat - \frac{P^\flat}{mc} \right\}. \tag{5.3.33}$$

Using this, we can show:

Lemma 5.3.11. *χ is a centre of spin* $\iff$ $\chi(u,\tau) - \chi^{\mathrm{NW}}(u,\tau) \in \operatorname{span}\{u, P\}$.

Proof. Writing $D := \chi(u,\tau) - \chi^{\mathrm{NW}}(u,\tau)$, the spin tensor of χ may be expressed as $S(u) = S^{\mathrm{NW}}(u) - D^\flat \wedge P^\flat$. Thus, (5.3.33) is equivalent to

$$\iota_{u+\frac{P}{mc}}(D^\flat \wedge P^\flat) \in \operatorname{span}\left\{u^\flat - \frac{P^\flat}{mc}\right\}. \tag{5.3.34}$$

We have $\iota_{u+\frac{P}{mc}}(D^\flat \wedge P^\flat) = (D \cdot u + \frac{D\cdot P}{mc})P^\flat - (P \cdot u - mc)D^\flat$, and thus (5.3.34) implies that for all $v \in u^\perp \cap P^\perp$, we have

$$v \cdot D = 0. \tag{5.3.35}$$

But this means $D \in (u^\perp \cap P^\perp)^\perp = \operatorname{span}\{u, P\}$.

Conversely, if $D \in \operatorname{span}\{u, P\}$, we have $\iota_{u+\frac{P}{mc}}(D^\flat \wedge P^\flat) \in \operatorname{span}\left\{\iota_{u+\frac{P}{mc}}(u^\flat \wedge P^\flat)\right\}$. But now

$$\iota_{u+\frac{P}{mc}}(u^\flat \wedge P^\flat) = \left(-1 + u \cdot \frac{P}{mc}\right)P^\flat - (u \cdot P - mc)u^\flat = (mc - u \cdot P)\left(u^\flat - \frac{P^\flat}{mc}\right), \tag{5.3.36}$$

and thus we have (5.3.34), i.e. χ is a centre of spin. $\square$

We can now prove the main result of this section.

Theorem 5.3.12. *The Newton–Wigner position observable χ^{NW} is the only centre of spin position observable that is continuous and defined by an* SSC.

Proof. Let χ be an SSC position observable. Writing $D(u,\tau) := \chi(u,\tau) - \chi^{\mathrm{NW}}(u,\tau)$, we know by the Møller disc theorem (theorem 5.3.6) that the projection of $D(u,\tau)$ orthogonal to P is orthogonal to the Pauli–Lubański vector W. Thus, since P itself is orthogonal to W, we have

$$D(u,\tau) \perp W \tag{5.3.37}$$

for any $(u,\tau) \in \mathrm{SpHP}$. In addition, we know that $D(u,\tau) \perp u$; in particular, $D(u,\tau)$ is spacelike for any $(u,\tau) \in \mathrm{SpHP}$.

Now suppose that χ is a centre of spin. By lemma 5.3.11 this means that

$$D(u,\tau) \in \operatorname{span}\{u, P\} \tag{5.3.38}$$

for all $(u,\tau) \in \mathrm{SpHP}$. Using (5.3.37) and $P \perp W$, we conclude that

$$\text{for all } u \text{ with } u \cdot W \neq 0 : D(u,\tau) \in \operatorname{span}\{P\}. \tag{5.3.39}$$

Since $D(u,\tau)$ has to be spacelike, we thus have shown

$$D(u,\tau) = 0 \text{ for all } u \text{ with } u \cdot W \neq 0. \tag{5.3.40}$$

If $W \neq 0$, the set of future-directed unit timelike u satisfying $u \cdot W \neq 0$ is dense in the hyperboloid of all possible u, and thus assuming continuity of χ, we conclude that $D(u, \tau) = 0$ for all u, finishing the proof.

If $W = 0$, then by the Møller disc theorem all SSC worldlines coincide, and thus we also have $\chi = \chi^{\mathrm{NW}}$. □

Looking back into the various steps of the proofs it is interesting to note how the 'extrinsic–intrinsic' combination $u + P/(mc)$ for f came about. It entered through the unique boost transformation (5.3.24) that was needed in order to transform an intrinsic quantity to an externally specified rest frame. The intrinsic quantity is the spin vector in the momentum rest frame, i.e. the Pauli–Lubański vector, which is a function of Γ only, and the externally specified frame is defined by u, which is independent of Γ and determined through the choice of $\Sigma \in \mathrm{SpHP}$.

5.4. A Newton–Wigner theorem for classical elementary systems

For elementary Poincaré-invariant quantum systems – i.e. quantum systems with an irreducible unitary action of the Poincaré group – the Newton–Wigner position operator is uniquely characterised by transforming 'as a position should' under translations, rotations and time reversal, having commuting components and satisfying a regularity condition. This has been well-known since the original publication by Newton and Wigner [NW49]. As advertised in the introduction, we shall now prove an analogous statement for classical systems.

For the whole of this section, we fix a future-directed unit timelike vector u defining a Lorentz frame, and an adapted positively oriented orthonormal basis $\{u = \mathrm{e}_0, \ldots, \mathrm{e}_3\}$. Unless otherwise stated, phrases such as 'temporal', 'spatial' and the like refer to the preferred time direction given by u. We will raise and lower spatial indices by the Euclidean metric δ induced by the Minkowski metric η on the orthogonal complement of u; the components of δ in the adapted basis are simply given by the usual Kronecker delta. We denote the spatial volume form by ${}^{(3)}\varepsilon = \iota_u \varepsilon$.

Similar to the notation introduced in chapter 2, we will employ a 'three-vector' notation for spatial vectors, for example writing $\boldsymbol{A} = (A^a)$. We then use the usual three-vector notations for the Euclidean scalar product $\boldsymbol{A} \cdot \boldsymbol{B} = A_a B^a$, the Euclidean norm $|\boldsymbol{A}| := \sqrt{\boldsymbol{A}^2}$ and the vector product $(\boldsymbol{A} \times \boldsymbol{B})_a = {}^{(3)}\varepsilon_{abc} A^b B^c$.

5.4.1. Classical elementary systems

In the quantum case, an elementary system is given by a Hilbert space with an *irreducible* unitary action of the Poincaré group – i.e. each state of the system is connected to any other by a Poincaré transformation. In direct analogy, we define the notion of a classical elementary system:

Definition 5.4.1. A *classical elementary system* is a classical Poincaré-invariant system (Γ, ω, Φ), where Φ is a transitive action of the proper orthochronous Poincaré group $\mathcal{P}_+^\uparrow$.

Note the we only assumed an action of the identity connected component of the Poincaré group, whereas Arens in [Are71b] considered the whole Poincaré group. In the classical context, simple transitivity replaces irreducibility in the quantum case.

Arens classified the classical elementary systems[11] in [Are71b]; the classification proceeds in terms of the system's four-momentum and Pauli–Lubański vector (similar to the Wigner classification in the quantum case [Wig39]). We are only interested in the case of timelike four-momentum. For this case, the phase space can be explicitly constructed as follows:

Theorem 5.4.2 (Phase space of a classical elementary system)**.** *Any classical elementary system with timelike four-momentum is equivalent (in the sense of a symplectic isomorphism respecting the action of $\mathcal{P}_+^\uparrow$) to precisely one of the following two cases:*

(i) (Spin zero, one parameter $m \in \mathbb{R}_+$)

- *Phase space $\Gamma = T^*\mathbb{R}^3$ with coordinates $(\boldsymbol{x}, \boldsymbol{p})$, symplectic form $\omega = \mathrm{d}x^a \wedge \mathrm{d}p_a$*
- *Poincaré generators (i.e. component functions of the momentum map):*

$$\begin{aligned} \textit{spatial translations} \quad & P_a = p_a && (5.4.1a) \\ \textit{time translation} \quad & P_0 = -\sqrt{m^2c^2 + \boldsymbol{p}^2} && (5.4.1b) \\ \textit{rotations} \quad & J_{ab} = x_a p_b - x_b p_a && (5.4.1c) \\ \textit{boosts} \quad & J_{a0} = P_0 x_a && (5.4.1d) \end{aligned}$$

(ii) (Spin non-zero, two parameters $m, S \in \mathbb{R}_+$)

[11] In fact, Arens classified what he called *one-particle* elementary systems (systems that admit a map from Γ to the set of lines in Minkowski space which is equivariant with respect to a certain subgroup of $\mathcal{P}_+^\uparrow$). However, he also proved that this 'one-particle' condition is fulfilled for an elementary system if and only if the four-momentum is not zero.

- *Phase space* $\Gamma = T^*\mathbb{R}^3 \times S^2$ *with coordinates* $(\boldsymbol{x}, \boldsymbol{p})$ *for* $T^*\mathbb{R}^3$*, symplectic form* $\omega = \mathrm{d}x^a \wedge \mathrm{d}p_a + S \cdot \mathrm{d}\Omega^2$ *where* $\mathrm{d}\Omega^2$ *is the standard volume form on* S^2*. We denote the phase space function projecting onto the second factor* S^2 *by* $\hat{\boldsymbol{s}} \colon \Gamma \to S^2 \subset \mathbb{R}^3$*. The* spin vector *observable is the* S^2_S*-valued phase space function* $\boldsymbol{s} := S \cdot \hat{\boldsymbol{s}}$*; its components satisfy the Poisson bracket relations*

$$\{s_a, s_b\} = {}^{(3)}\varepsilon_{abc} s^c. \tag{5.4.2}$$

  Here $S^2_S \subset \mathbb{R}^3$ *denotes the 2-sphere of radius* S *in* $\mathbb{R}^3$*.*
- *Poincaré generators (i.e. component functions of the momentum map):*

$$\text{spatial translations} \quad P_a = p_a \tag{5.4.3a}$$

$$\text{time translation} \quad P_0 = -\sqrt{m^2c^2 + \boldsymbol{p}^2} \tag{5.4.3b}$$

$$\text{rotations} \quad J_{ab} = x_a p_b - x_b p_a + {}^{(3)}\varepsilon_{abc} s^c \tag{5.4.3c}$$

$$\text{boosts} \quad J_{a0} = P_0 x_a - \frac{(\boldsymbol{p} \times \boldsymbol{s})_a}{mc - P_0} \tag{5.4.3d}$$

Note that in fact the explicit construction of the systems in [Are71b] as co-adjoint orbits of $\mathcal{P}^\uparrow_+$ is quite different in appearance to the forms given above. However, one can show that the above systems are indeed elementary systems (i.e. that the action of $\mathcal{P}^\uparrow_+$ is transitive), and thus due to Arens' uniqueness result they are possible representatives of their respective classes. We will use the forms given above, which were anticipated by Bacry in [Bac67], since they will be easier to explicitly work with. To unify notation, we let $S = 0, \boldsymbol{s} := 0$ in the case of zero-spin systems. Furthermore, we introduce the open subset of phase space $\Gamma^* := \Gamma \setminus \{|\boldsymbol{P}| = 0\}$ and the S^2-valued function $\hat{\boldsymbol{P}} := \frac{\boldsymbol{P}}{|\boldsymbol{P}|}$ on Γ^*.

Using the explicit form of the systems given in theorem 5.4.2, one directly checks:

Lemma 5.4.3. *For a classical elementary system with timelike four-momentum, the functions* $P_a, \hat{\boldsymbol{P}} \cdot \boldsymbol{s}$ *(or just the* P_a *in the case of zero spin) form a complete involutive set on* Γ^* *(or the whole of* Γ *in the case of zero spin).* □

The behaviour of the momentum and spin vectors under translations and rotations is also easily obtained:

Lemma 5.4.4. *For a classical elementary system with timelike four-momentum,* $\boldsymbol{P}$ *and* $\boldsymbol{s}$ *are invariant under translations and 'transform as vectors' under spatial rotations, i.e. we have*

$$\{P_a, V_b\} = 0, \quad \{J_{ab}, V_c\} = \delta_{ac} V_b - \delta_{bc} V_a \quad \text{for} \quad \boldsymbol{V} = \boldsymbol{P}, \boldsymbol{s}. \tag{5.4.4}$$

Proof. For $\boldsymbol{P}$, these are part of the Poincaré algebra relations and thus true by definition. For $\boldsymbol{s}$, they are easily confirmed using the explicit form of the Poincaré generators. □

For our considerations, we will need to know how the *time reversal* operation with respect to the hyperplane in M through the origin $o \in M$ and orthogonal to $u = \mathrm{e}_0$ is implemented on phase space. In order to get this right, we recall that the incorporation of time reversal in the context of special relativity corresponds, by its very definition, to a particular upward $\mathbb{Z}_2$ extension[12] of $\mathcal{P}_+^\uparrow$, i.e. the formation of a new group called $\mathcal{P}_+^\uparrow \cup \mathcal{P}_-^\downarrow$ of which $\mathcal{P}_+^\uparrow$ is a normal subgroup with $(\mathcal{P}_+^\uparrow \cup \mathcal{P}_-^\downarrow)/\mathcal{P}_+^\uparrow \cong \mathbb{Z}_2$. It is the particular nature of this extension that eventually defines what is meant by *time reversal*: it consists in the requirement that the outer automorphism induced by the only non-trivial element of $\mathbb{Z}_2$ on the Lie algebra $\mathfrak{p}$ of $\mathcal{P}_+^\uparrow$ shall be the one which reverses the sign of spatial translations and rotations and leaves invariant boosts and time translations; see, e.g., [BL68]. Implementing time reversal on phase space then means to extend the action of $\mathcal{P}_+^\uparrow$ to an action of $\mathcal{P}_+^\uparrow \cup \mathcal{P}_-^\downarrow$.

Now, according to this scheme, we can immediately write down how our particular time reversal transformation on phase space, $T_u \colon \Gamma \to \Gamma$, acts on the Poincaré generators, i.e. the component functions of the momentum map:

$$P_a \circ T_u = -P_a \,, \quad J_{ab} \circ T_u = -J_{ab} \,, \quad J_{a0} \circ T_u = J_{a0} \,, \quad P_0 \circ T_u = P_0 \tag{5.4.5}$$

From this the well-known result follows that time reversal (as defined above) necessarily corresponds to an *anti*-symplectomorphism (inverting the sign of the symplectic form). Hence, in the process of extending our symplectic action of $\mathcal{P}_+^\uparrow$ on Γ to an action of $\mathcal{P}_+^\uparrow \cup \mathcal{P}_-^\downarrow$ satisfying the time reversal criterion above, we had to generalise to possibly *anti*-symplectomorphic actions. This is akin to the situation in quantum mechanics, where, as is well-known, time reversal necessarily corresponds to an *anti*-unitary transformation.

It is now clear how time reversal is implemented in the case at hand:

Lemma 5.4.5. *For an elementary system as in theorem 5.4.2, time reversal with respect to the hyperplane through the origin and orthogonal to $u = \mathrm{e}_0$ is given by*

$$T_u \colon (\boldsymbol{x}, \boldsymbol{p}, \hat{\boldsymbol{s}}) \mapsto (\boldsymbol{x}, -\boldsymbol{p}, -\hat{\boldsymbol{s}}). \tag{5.4.6}$$

□

Unless otherwise stated, in the following we will always mean time reversal with respect to the hyperplane through the origin and orthogonal to $u = \mathrm{e}_0$ when saying 'time reversal'.

[12] Here we are using the terminology of [Con+85, p. xx], according to which a group G with normal subgroup A and quotient $G/A \cong B$ is either called an *upward extension* of A by B or a *downward extension* of B by A.

5.4.2. Statement and interpretation of the Newton–Wigner theorem

The classical Newton–Wigner theorem we are going to prove can be formulated very similar to the quantum case:

Theorem 5.4.6 (Classical Newton–Wigner theorem)**.** *For a classical elementary system with timelike four-momentum, there is a unique $\mathbb{R}^3$-valued phase space function $\boldsymbol{X}$ that*

(i) is C^1,

(ii) has Poisson-commuting components,

(iii) satisfies the canonical Poisson relations $\{X^a, P_b\} = \delta^a_b$ with the generators of spatial translations with respect to $u = \mathrm{e}_0$,

(iv) transforms 'as a (position) vector' under spatial rotations with respect to $u = \mathrm{e}_0$, i.e. satisfies $\{J_{ab}, X^c\} = \delta^c_a X_b - \delta^c_b X_a$, and

(v) is invariant under time reversal with respect to the hyperplane through the origin and orthogonal to $u = \mathrm{e}_0$, i.e. satisfies $\boldsymbol{X} \circ T_u = \boldsymbol{X}$.

In terms of the Poincaré generators, it is given by

$$X_a = -\frac{J_{a0}}{mc} - \frac{J_{ab}P^b}{mc(mc - P_0)} - \frac{J_{b0}P^b}{P_0 mc(mc - P_0)} P_a \,, \tag{5.4.7}$$

where $m = \sqrt{P_0^2 - \boldsymbol{P}^2}/c$ is the mass of the system.

Before proving the theorem in the next section, we will now discuss the interpretation of the 'position' $\boldsymbol{X}$ it characterises. We want to interpret the value of $\boldsymbol{X}$ (in some state $\gamma \in \Gamma$) as the spatial components of a point in Minkowski spacetime M. Since $\boldsymbol{X}$ is invariant under time reversal with respect to the hyperplane through the origin and orthogonal to $u = \mathrm{e}_0$, it can be interpreted as defining a point on this hyperplane. Thus, if we want to use the phase space function from the Newton–Wigner theorem to define a position observable χ in the sense of section 5.3.1, we should set (in our basis adapted to u)

$$\chi^a(u, \tau = 0) := X^a \,, \quad \chi^0(u, \tau = 0) := 0. \tag{5.4.8}$$

The transformation behaviour of $\boldsymbol{X}$ under spatial translations and rotations (i.e. assumptions (iii) and (iv) of theorem 5.4.6) will then ensure that the position observable χ be covariant (in the sense of definition 5.3.2) regarding these transformations.

In fact, comparing (5.4.7) to the expression (5.3.17) for the Newton–Wigner position observable χ^{NW}, we see that we have (in our adapted basis)

$$\chi^{\mathrm{NW},a}(u, \tau = 0) = X^a \,, \quad \chi^{\mathrm{NW},0}(u, \tau = 0) = 0: \tag{5.4.9}$$

the position $\boldsymbol{X}$ characterised by theorem 5.4.6 is the one given by the Newton–Wigner position observable χ^{NW} on the hyperplane $(u, 0) \in \mathrm{SpHP}$ (which is a covariant position observable due to proposition 5.3.5). Let us also remark that since any position observable's dependence on τ is fixed by (5.3.8), a position observable satisfying (5.4.8) is equal to the Newton–Wigner observable χ^{NW} on the whole family of hyperplanes $\Sigma \in \mathrm{SpHP}$ with normal vector u.

Combining this identification with the observation that we can freely choose the origin $o \in M$, we can restate the Newton–Wigner theorem in the following form:

Theorem 5.4.7 (Classical Newton–Wigner theorem, version 2)**.** *For a classical elementary system with timelike four-momentum, given any hyperplane $\Sigma = (u, \tau) \in \mathrm{SpHP}$, there is a unique Σ-valued phase space function $\chi^{\mathrm{NW}}(\Sigma)$ that*

(i) is C^1,

(ii) has Poisson-commuting components, i.e.

$$\left\{\chi^{\mathrm{NW},\mu}(\Sigma), \chi^{\mathrm{NW},\nu}(\Sigma)\right\} = 0, \tag{5.4.10a}$$

(iii) satisfies the canonical Poisson relations with the generators of spatial translations with respect to u, i.e.

$$v_\mu w^\nu \left\{\chi^{\mathrm{NW},\mu}(\Sigma), P_\nu\right\} = v \cdot w \text{ for } v, w \in u^\perp, \tag{5.4.10b}$$

(iv) transforms 'as a position' under spatial rotations with respect to u, i.e. satisfies

$$v^\mu \tilde{v}^\nu w_\rho \left\{J_{\mu\nu}, \chi^{\mathrm{NW},\rho}(\Sigma)\right\} = v^\mu \tilde{v}^\nu w_\rho \left[\delta^\rho_\mu \chi^{\mathrm{NW}}_\nu(\Sigma) - \delta^\rho_\nu \chi^{\mathrm{NW}}_\mu(\Sigma)\right] \text{ for } v, \tilde{v}, w \in u^\perp, \tag{5.4.10c}$$

and

(v) is invariant under time reversal with respect to Σ.

These $\chi^{\mathrm{NW}}(\Sigma)$ together form the Newton–Wigner observable as given by (5.3.17). □

5.4.3. Proof of the Newton–Wigner theorem

Proof of theorem 5.4.6. For the whole of the proof, we will work with the explicit form of the phase space of our elementary system given in theorem 5.4.2. It is easily verified that in this explicit form, $\boldsymbol{x}$ (i.e. the coordinate of the base point in $T^*\mathbb{R}^3$) is a phase space function with the properties demanded for $\boldsymbol{X}$. Thus we need to prove uniqueness. Our proof will follow the proof of the quantum-mechanical Newton–Wigner theorem given by Jordan in [Jor80], some parts of which can be applied literally to the classical case.

We will several times need the following.

Lemma 5.4.8. *Consider a classical elementary system with timelike four-momentum, with phase space* Γ*, and some open subset* $\tilde{\Gamma}$ *of* $\Gamma^* = \Gamma \setminus \{|\boldsymbol{P}| = 0\}$*. Let* f *be an* $\mathbb{R}$*-valued* C^1 *function defined on* $\tilde{\Gamma}$ *that is invariant under spatial translations and rotations, i.e.* $\{P_a, f\} = 0 = \{J_{ab}, f\}$*. Then* f *is a function of* $|\boldsymbol{P}|, \hat{\boldsymbol{P}} \cdot \boldsymbol{s}$*.* [13]

Proof. f Poisson-commutes with $\boldsymbol{P}$ and J_{ab}. Therefore it also Poisson-commutes with $\boldsymbol{P}$ and $\frac{1}{2}{}^{(3)}\varepsilon^{abc}\hat{P}_a J_{bc} = \hat{\boldsymbol{P}} \cdot \boldsymbol{s}$. Now $\boldsymbol{P}, \hat{\boldsymbol{P}} \cdot \boldsymbol{s}$ form a complete involutive set on Γ^* (lemma 5.4.3), so since f Poisson-commutes with them, it must be a function of $\boldsymbol{P}, \hat{\boldsymbol{P}} \cdot \boldsymbol{s}$. Since f and $\hat{\boldsymbol{P}} \cdot \boldsymbol{s}$ are rotation invariant (by lemma 5.4.4), f must be a function of $|\boldsymbol{P}|, \hat{\boldsymbol{P}} \cdot \boldsymbol{s}$. □

Let now $\boldsymbol{X}$ be an observable as in the statement of theorem 5.4.6, and consider the difference $\boldsymbol{d} := \boldsymbol{X} - \boldsymbol{x}$. Due to the assumptions of theorem 5.4.6, $\boldsymbol{d}$ is C^1, is invariant under translations (i.e. $\{d^a, P_b\} = 0$), transforms as a vector under spatial rotations (i.e. $\{J_{ab}, d^c\} = \delta^c_a d_b - \delta^c_b d_a$) and is invariant under time reversal with respect to the hyperplane through the origin and orthogonal to u (i.e. $\boldsymbol{d} \circ T_u = \boldsymbol{d}$).

Lemma 5.4.9. *Let* $\boldsymbol{A}$ *be a* $\mathbb{R}^3$*-valued* C^1 *phase space function on a classical elementary system with timelike four-momentum that is invariant under translations, transforms as a vector under spatial rotations and is invariant under time reversal. Then* $\boldsymbol{A} \cdot \boldsymbol{P} = 0$*.*

Proof. Since $\boldsymbol{P}$ is invariant under translations and a vector under rotations, $\boldsymbol{A} \cdot \boldsymbol{P}$ is invariant under translations and rotations. By lemma 5.4.8, $\boldsymbol{A} \cdot \boldsymbol{P}|_{\Gamma^*}$ is a function of $|\boldsymbol{P}|, \hat{\boldsymbol{P}} \cdot \boldsymbol{s}$. This means we have

$$\boldsymbol{A} \cdot \boldsymbol{P}|_{\Gamma^*} = F(|\boldsymbol{P}|, \hat{\boldsymbol{P}} \cdot \boldsymbol{s}) \tag{5.4.11}$$

for some function $F\colon \mathbb{R}_+ \times [-S, S] \to \mathbb{R}$.

Now considering time reversal T_u, on the one hand we have (using lemma 5.4.5)

$$|\boldsymbol{P}| \circ T_u = |\boldsymbol{P} \circ T_u| = |-\boldsymbol{P}| = |\boldsymbol{P}| \tag{5.4.12a}$$

[13] By 'f is a function of $|\boldsymbol{P}|, \hat{\boldsymbol{P}} \cdot \boldsymbol{s}$' we mean that f depends on phase space only via $|\boldsymbol{P}|, \hat{\boldsymbol{P}} \cdot \boldsymbol{s}$, i.e. that there is a C^1 function $F\colon U \to \mathbb{R}$, $U = \{(|\boldsymbol{P}|(\gamma), (\hat{\boldsymbol{P}} \cdot \boldsymbol{s})(\gamma)) : \gamma \in \tilde{\Gamma}\} \subset \mathbb{R}_+ \times [-S, S]$ satisfying

$$f(\gamma) = F(|\boldsymbol{P}|(\gamma), (\hat{\boldsymbol{P}} \cdot \boldsymbol{s})(\gamma)) \text{ for all } \gamma \in \tilde{\Gamma}.$$

and

$$
\begin{aligned}
(\hat{\boldsymbol{P}} \cdot \boldsymbol{s}) \circ T_u &= \left(\frac{1}{2} {}^{(3)}\varepsilon^{abc} \hat{P}_a J_{bc} \right) \circ T_u \\
&= \frac{1}{2} {}^{(3)}\varepsilon^{abc} (\hat{P}_a \circ T_u)(J_{bc} \circ T_u) \\
&= \frac{1}{2} {}^{(3)}\varepsilon^{abc} (-\hat{P}_a)(-J_{bc}) \\
&= \frac{1}{2} {}^{(3)}\varepsilon^{abc} \hat{P}_a J_{bc} \\
&= \hat{\boldsymbol{P}} \cdot \boldsymbol{s},
\end{aligned}
\tag{5.4.12b}
$$

implying

$$
F(|\boldsymbol{P}|, \hat{\boldsymbol{P}} \cdot \boldsymbol{s}) \circ T_u = F(|\boldsymbol{P}| \circ T_u, (\hat{\boldsymbol{P}} \cdot \boldsymbol{s}) \circ T_u) = F(|\boldsymbol{P}|, \hat{\boldsymbol{P}} \cdot \boldsymbol{s}). \tag{5.4.13}
$$

On the other hand, $\boldsymbol{A}$ is invariant under time reversal while $\boldsymbol{P}$ changes its sign, implying that $(\boldsymbol{A} \cdot \boldsymbol{P}) \circ T_u = -\boldsymbol{A} \cdot \boldsymbol{P}$. Combining this with (5.4.11) and (5.4.13), we obtain $\boldsymbol{A} \cdot \boldsymbol{P}|_{\Gamma^*} = 0$, and continuity implies $\boldsymbol{A} \cdot \boldsymbol{P} = 0$. □

For zero spin, we can easily complete the proof of the Newton–Wigner theorem. Since the difference vector $\boldsymbol{d}$ is translation invariant and the P_a form a complete involutive set on Γ, $\boldsymbol{d}$ must be a function of $\boldsymbol{P}$. Then since it is a vector under rotations, it must be of the form

$$
\boldsymbol{d}(\boldsymbol{P}) = F(|\boldsymbol{P}|)\boldsymbol{P} \tag{5.4.14}
$$

for some function F of $|\boldsymbol{P}|$. Then, since according to lemma 5.4.9 $\boldsymbol{d} \cdot \boldsymbol{P}$ is zero, $\boldsymbol{d}$ is zero. Thus, for the spin-zero case, we have proved the Newton–Wigner theorem without any use of the condition of Poisson-commuting components of the position observable.

For the non-zero spin case, we continue as follows.

Lemma 5.4.10. *Let $\boldsymbol{A}$ be a $\mathbb{R}^3$-valued C^1 phase space function on a classical elementary system with timelike four-momentum and non-zero spin that is invariant under translations, transforms as a vector under spatial rotations and satisfies $\boldsymbol{A} \cdot \boldsymbol{P} = 0$. Then it is of the form*

$$
\boldsymbol{A} = B\hat{\boldsymbol{P}} \times \boldsymbol{s} + C\hat{\boldsymbol{P}} \times (\hat{\boldsymbol{P}} \times \boldsymbol{s}) \tag{5.4.15}
$$

on $\Gamma^* \setminus \{\boldsymbol{s} \parallel \hat{\boldsymbol{P}}\}$, where B and C are C^1 functions of $|\boldsymbol{P}|$ and $\hat{\boldsymbol{P}} \cdot \boldsymbol{s}$, i.e. C^1 functions

$$
B, C \colon \mathbb{R}_+ \times (-S, S) \to \mathbb{R}.
$$

Proof. For the whole of this proof, we will work on $\tilde{\Gamma} := \Gamma^* \setminus \{\boldsymbol{s} \parallel \hat{\boldsymbol{P}}\}$. Since evaluated at each point of $\tilde{\Gamma}$, the $\mathbb{R}^3$-valued functions $\hat{\boldsymbol{P}}, \hat{\boldsymbol{P}} \times \boldsymbol{s}, \hat{\boldsymbol{P}} \times (\hat{\boldsymbol{P}} \times \boldsymbol{s})$ form an orthogonal basis of $\mathbb{R}^3$, and since we have $\boldsymbol{A} \cdot \boldsymbol{P} = 0$, we can write $\boldsymbol{A}$ in the form (5.4.15) with coefficients B, C given by

$$B = \frac{\boldsymbol{A} \cdot (\hat{\boldsymbol{P}} \times \boldsymbol{s})}{|\hat{\boldsymbol{P}} \times \boldsymbol{s}|}\,, \tag{5.4.16}$$

$$C = \frac{\boldsymbol{A} \cdot (\hat{\boldsymbol{P}} \times (\hat{\boldsymbol{P}} \times \boldsymbol{s}))}{|\hat{\boldsymbol{P}} \times (\hat{\boldsymbol{P}} \times \boldsymbol{s})|}\,. \tag{5.4.17}$$

Since $\boldsymbol{A}$, $\boldsymbol{P}$ and $\boldsymbol{s}$ are invariant under translations and vectors under rotations, these equations imply that B, C are invariant under translations and rotations. The result follows with lemma 5.4.8. □

Now we consider again the difference vector $\boldsymbol{d} = \boldsymbol{X} - \boldsymbol{x}$. It satisfies $\boldsymbol{d} \cdot \boldsymbol{P} = 0$ by lemma 5.4.9, and thus we have

$$\boldsymbol{X} \cdot \boldsymbol{P} = \boldsymbol{x} \cdot \boldsymbol{P}. \tag{5.4.18}$$

Since we assume that the components of $\boldsymbol{X}$ Poisson-commute with each other and that $\{X^a, P_b\} = \delta^a_b$, this implies

$$\{X^a, \boldsymbol{x} \cdot \boldsymbol{P}\} = \{X^a, \boldsymbol{X} \cdot \boldsymbol{P}\} = X^a. \tag{5.4.19}$$

Combining this with $\{x^a, \boldsymbol{x} \cdot \boldsymbol{P}\} = x^a$, we obtain

$$\{d^a, \boldsymbol{x} \cdot \boldsymbol{P}\} = d^a. \tag{5.4.20}$$

On the other hand, for any function F of $\boldsymbol{P}$ and $\boldsymbol{s}$, we have

$$\{F(\boldsymbol{P}, \boldsymbol{s}), \boldsymbol{x} \cdot \boldsymbol{P}\} = \{F(\boldsymbol{P}, \boldsymbol{s}), x^a\} P_a = -\frac{\partial F(\boldsymbol{P}, \boldsymbol{s})}{\partial P_a} P_a = -|\boldsymbol{P}| \left.\frac{\partial F}{\partial |\boldsymbol{P}|}\right|_{\hat{\boldsymbol{P}}=\text{const.}, \boldsymbol{s}=\text{const.}}. \tag{5.4.21}$$

This implies

$$\boldsymbol{d} = -|\boldsymbol{P}| \left.\frac{\partial \boldsymbol{d}}{\partial |\boldsymbol{P}|}\right|_{\hat{\boldsymbol{P}}=\text{const.}, \boldsymbol{s}=\text{const.}}. \tag{5.4.22}$$

Combining lemmas 5.4.9 and 5.4.10, we know that $\boldsymbol{d}$ has the form (5.4.15) on $\Gamma^* \setminus \{\boldsymbol{s} \parallel \hat{\boldsymbol{P}}\}$ for two functions $B, C \colon \mathbb{R}_+ \times (-S, S) \to \mathbb{R}$. Thus (5.4.22) implies the two equations

$$B(|\boldsymbol{P}|, \hat{\boldsymbol{P}} \cdot \boldsymbol{s}) = -|\boldsymbol{P}| \frac{\partial B(|\boldsymbol{P}|, \hat{\boldsymbol{P}} \cdot \boldsymbol{s})}{\partial |\boldsymbol{P}|},\ C(|\boldsymbol{P}|, \hat{\boldsymbol{P}} \cdot \boldsymbol{s}) = -|\boldsymbol{P}| \frac{\partial C(|\boldsymbol{P}|, \hat{\boldsymbol{P}} \cdot \boldsymbol{s})}{\partial |\boldsymbol{P}|} \tag{5.4.23}$$

on $\mathbb{R}_+ \times (-S, S)$. These equations determine the $|\boldsymbol{P}|$ dependence of B and C; they must be proportional to $|\boldsymbol{P}|^{-1}$. However, for $\boldsymbol{d}$ to be C^1 on the whole of Γ, in fact for (5.4.15) not to diverge as $|\boldsymbol{P}| \to 0$ even when coming from a *single* direction $\hat{\boldsymbol{P}}$, we then need B and C to vanish. Continuity implies $\boldsymbol{d} = 0$ on all of Γ. This finishes the proof of the Newton–Wigner theorem. □

5.5. Conclusion

In this chapter we have studied the localisation problem for classical system whose phase space is a symplectic manifold. We focussed on the Newton–Wigner position observable and asked for precise characterisations of it in order to gain additional understanding, over and above that already known from its practical use for the solution of concrete problems of motion, e.g., in general-relativistic astrophysics [Ste11; SJ18]. We proved two theorems that we believe advance our understanding in the desired direction: first we showed how Fleming's geometric scheme [Fle65] in combination with the characterisation of worldlines through SSCs (Spin Supplementary Conditions) allows to give a precise meaning to, and proof of, the fact that the Newton–Wigner position is the unique centre of spin. Given that interpretation, it also offers an insight as to why the Newton–Wigner SSC uses a somewhat unnatural looking 'hybrid' combination $f = u + \frac{P}{mc}$, where u is 'external' or 'kinematical', and P is 'internal' or 'dynamical'. Then, restricting to elementary systems, i.e. systems whose phase space admits a transitive action of the proper orthochronous Poincaré group, we proved again a uniqueness result to the effect that the Newton–Wigner observable is the unique phase space function whose components satisfy the 'familiar' Poisson relations, provided it is continuously differentiable, time-reversal invariant, and transforms as a vector under spatial rotations. These properties seem to be the underlying reason for the distinguished rôle it plays in solution strategies like those of [Ste11; SJ18], despite the fact that on a more general level of theorisation other choices (characterised by other SSCs) are often considered more appropriate; see, e.g., [PLS15]. We believe that our results add a conceptually clear and mathematically precise Hamiltonian underpinning of what the choice of the Newton–Wigner observable entails, at least in a special-relativistic context or, more generally, in general-relativistic perturbation theory around Minkowski space.

6. Conclusion

In this thesis, we have developed and analysed systematic methods for the description of quantum-mechanical systems to post-Newtonian gravitational fields. As explained in the introduction, we see the virtue of our systematic calculations in their firm rooting in explicitly spelled out principles, that leave no doubt concerning the questions of consistency and completeness of the obtained 'relativistic corrections'. This, in our opinion, distinguishes our work from previous ones by other authors, who were also concerned with the coupling of composite particle quantum systems – like atoms or molecules – to external gravitational fields, who phrase their account of 'relativistic corrections' in terms of semi-classical notions, like smooth worldlines and comparisons of their associated lengths (i.e. 'proper time' and 'redshift'); e.g. [Dim+08; Zyc+11; Pik+15; Rou18; Gie+19; Lor+19; ZRP19]. In our opinion, answers to the fundamental question of gravity–matter coupling in quantum mechanics should not be based on *a priori* restricted states that imply a semi-classical behaviour of some of the (factorising) degrees of freedom. Rather, they should apply to all states in an equally valid fashion.

In chapter 3, we have shown how to systematically derive a Schrödinger equation with post-Newtonian correction terms describing a single quantum particle in a general post-Newtonian curved background spacetime by means of a WKB-like formal expansion of the minimally coupled Klein–Gordon equation. We extended this method to account for, in principle, post-Newtonian terms of arbitrary orders in c^{-1}, although it gets recursive at higher orders, making it computationally more difficult to handle than methods based on formal quantisation of the classical description of the particle. Nevertheless, we believe this scheme to be better suited for concrete predictions, since it is more firmly based on first principles and also more systematic than *ad hoc* canonical quantisation or path integral procedures as employed widely in the literature. For example, no operator ordering ambiguities arise; instead, the WKB method can be seen as *predicting* the ordering.

Comparing the Klein–Gordon expansion method to canonical quantisation, we have found that in the case of a general metric, even at lowest post-Newtonian order, the two procedures lead to slightly different quantum Hamiltonians, *independent of ordering ambiguities*[1]. For the concrete case of the metric of the Eddington–Robertson PPN test

[1]At least if only simple symmetrising procedures are allowed for as ordering schemes in canonical quantisation, see the discussion at the end of section 3.4.2.

theory, the Hamiltonians obtained from the two methods differ in a term including the Eddington–Robertson parameter γ, depending on the ordering scheme employed in canonical quantisation. Although the relevant term is proportional to the Laplacian of the Newtonian potential, i.e. (in lowest order) to the mass density generating the gravitational field, and thus is irrelevant in physical situations concerning the *outside* of the generating matter distribution, this example shows that for the interpretation of tests of general relativity with quantum systems, the method used to derive the quantum Hamiltonian plays a decisive rôle.

For the case of stationary background metrics, without employing any expansion of the metric, we showed that up to linear order in spatial momenta, the Hamiltonians obtained from canonical quantisation and from the Klein–Gordon equation agree. In particular, this means that the lowest-order coupling to the 'gravitomagnetic' field components g^{0a} is independent of the gravity–quantum matter coupling method.

Concerning the applicability of the WKB-like expansion method for concrete calculations, it could be an interesting question for future research if and how the transformation of the Hamiltonian from the Klein–Gordon inner product to an L^2-scalar product – be it flat or with respect to the induced metric measure – can be implemented more systematically, not relying on direct calculations with the already-computed Hamiltonian.

Turning to the description of composite systems, in chapter 4 we extended the calculation of [SB18] of a Hamiltonian describing an electromagnetically interacting two-particle system so as to include post-Newtonian gravity as described by the Eddington–Robertson PPN metric. Starting from first principles, we performed a post-Newtonian expansion in terms of the inverse velocity of light that led to leading-order corrections comprising special- and general-relativistic effects. The former were fully encoded in [SB18], but the latter are new. As in [SB18] we neglected all terms of third and higher order in c^{-1}, which physically means that we neglected radiation-reaction and also that we avoided obstructions on the applicability of the Hamiltonian formalism that result from the infamous 'no-interaction theorem' [CJS63; SM16], whose impact only starts at the 6th order in a c^{-1} expansion [MS78].

Similar to the gravity-free case, we now *derived* the result that the centre of mass motion of the system can be viewed as that of a 'composite point particle', including in its mass the internal energy of the system. This result may be anticipated in a heuristic fashion on semi-classical grounds, but, as seen, its proper derivation requires some efforts. We stress once more that for this interpretation it was crucial to express the Hamiltonian in terms of the physical space-time metric. As a result, our work lends some justification to current experimental proposals in atom interferometry that so far were based on these heuristic ideas, on the basis of which completeness of the relativistic effects could not be reliably judged; e.g. [Zyc+11; Pik+15; Rou18; Gie+19; Lor+19; ZRP19].

However, in order to obtain a fully solid framework for the discussion of atom interferometry in post-Newtonian gravity, stopping at the Hamiltonian is not enough: one has to describe the whole experimental situation solely in terms of operationally defined quantities. Such a systematic operational analysis of atom interferometers under gravity, which is now possible based on the Hamiltonian we obtained, we see as the most important future application of the results of this thesis. This may lead to interesting new possibilities of testing gravitational effects with quantum systems: in particular it might enable the measuring of post-Newtonian parameters, i.e. proper tests of general relativity, with laboratory experiments.

A. Calculation of the classical Hamiltonian of a free particle

Here, we will give a full exposition of the calculation of the classical Hamiltonian of a free particle in a curved spacetime in $3+1$ decomposition.

In $3+1$ decomposition, spacetime is foliated into three-dimensional spacelike Cauchy surfaces that are labelled by a 'foliation parameter' t. We employ adapted coordinates $(x^0 = ct, x^a)$ where x^a are coordinates on these Cauchy surfaces. This gives a decomposition of the spacetime metric as

$$g_{ab} = {}^{(3)}g_{ab}, \quad g_{0a} = {}^{(3)}g_{ab}\beta^b =: \beta_a, \quad g_{00} = -\alpha^2 + {}^{(3)}g_{ab}\beta^a\beta^b \;, \tag{A.1}$$

where ${}^{(3)}g$ is the induced metric on the Cauchy surfaces, β is the shift vector field and α is the lapse function. Geometrically speaking, lapse and shift arise from decomposing the 'time evolution' vector field[1] $\partial_0 = c^{-1}\partial/\partial t$ into its components tangential and normal to the Cauchy surfaces as

$$\frac{1}{c}\frac{\partial}{\partial t} = \alpha n + \beta, \tag{A.2}$$

where n is the future-directed unit normal to the Cauchy surfaces and β is the tangential component [Giu14, (17.44)].

Parametrising the worldline of a free particle by t, its Lagrangian (compare the classical action (3.2.1)) in these coordinates is

$$L = -mc\sqrt{-g_{\mu\nu}\dot{x}^\mu\dot{x}^\nu} = -mc\left(\alpha^2c^2 - {}^{(3)}g_{ab}\beta^a\beta^b c^2 - 2c\,{}^{(3)}g_{ab}\dot{x}^a\beta^b - {}^{(3)}g_{ab}\dot{x}^a\dot{x}^b\right)^{1/2}, \tag{A.3}$$

where a dot denotes differentiation with respect to t.

[1] Denoting the embeddings defining the foliation as $\mathcal{E}_t \colon \Sigma \to M,\ t \in \mathbb{R}$ where Σ is the abstract Cauchy surface, the time evolution vector field is given as the derivation

$$\left.\frac{\partial}{\partial t}\right|_{\mathcal{E}_s(q)} f := \left.\frac{\mathrm{d}}{\mathrm{d}s'} f(\mathcal{E}_{s'}(q))\right|_{s'=s}$$

for $q \in \Sigma$, $s \in \mathbb{R}$ and $f \in C^\infty(M)$; i.e. this vector field is independent of the choice of coordinates and depends just on the foliation, even if it was expressed above as a coordinate vector field. [Giu14, (17.43)]

From this, we compute the momentum p_a conjugate to x^a to be

$$p_a = \frac{\partial L}{\partial \dot{x}^a} = \frac{mc}{(\ldots)^{1/2}}(c\beta_a + {}^{(3)}g_{ab}\dot{x}^b). \tag{A.4}$$

Contracting with the inverse ${}^{(3)}g^{ab}$ of ${}^{(3)}g_{ab}$, we obtain

$$\dot{x}^a = \frac{(\ldots)^{1/2}}{mc}\,{}^{(3)}g^{ab}p_b - c\beta^a\,. \tag{A.5}$$

To fully express the velocity $\dot{x}^a$ in terms of the momentum p_a, we have to express $(\ldots)^{1/2} = \left(\alpha^2c^2 - {}^{(3)}g(\dot{\boldsymbol{x}} + c\boldsymbol{\beta}, \dot{\boldsymbol{x}} + c\boldsymbol{\beta})\right)^{1/2}$ in terms of p_a. Using (A.5), we have

$$\begin{aligned} {}^{(3)}g(\dot{\boldsymbol{x}} + c\boldsymbol{\beta}, \dot{\boldsymbol{x}} + c\boldsymbol{\beta}) &= \frac{(\ldots)}{m^2c^2}\,{}^{(3)}g^{ab}p_ap_b \\ &= \frac{\alpha^2c^2 - {}^{(3)}g(\dot{\boldsymbol{x}} + c\boldsymbol{\beta}, \dot{\boldsymbol{x}} + c\boldsymbol{\beta})}{m^2c^2}\,{}^{(3)}g^{ab}p_ap_b\,. \end{aligned} \tag{A.6}$$

Writing ${}^{(3)}g^{-1}(\boldsymbol{p}, \boldsymbol{p}) := {}^{(3)}g^{ab}p_ap_b$, this is equivalent to

$$\begin{aligned} {}^{(3)}g(\dot{\boldsymbol{x}} + c\boldsymbol{\beta}, \dot{\boldsymbol{x}} + c\boldsymbol{\beta}) &= \frac{\alpha^2\,{}^{(3)}g^{-1}(\boldsymbol{p}, \boldsymbol{p})}{m^2}\,\frac{1}{1 + {}^{(3)}g^{-1}(\boldsymbol{p}, \boldsymbol{p})/(m^2c^2)} \\ &= \frac{c^2\alpha^2\,{}^{(3)}g^{-1}(\boldsymbol{p}, \boldsymbol{p})}{m^2c^2 + {}^{(3)}g^{-1}(\boldsymbol{p}, \boldsymbol{p})} \end{aligned} \tag{A.7}$$

Using this, we get

$$(\ldots)^{1/2} = \left(\alpha^2c^2 - \frac{c^2\alpha^2\,{}^{(3)}g^{-1}(\boldsymbol{p}, \boldsymbol{p})}{m^2c^2 + {}^{(3)}g^{-1}(\boldsymbol{p}, \boldsymbol{p})}\right)^{1/2} = \frac{mc^2\alpha}{\left[m^2c^2 + {}^{(3)}g^{-1}(\boldsymbol{p}, \boldsymbol{p})\right]^{1/2}}\,. \tag{A.8}$$

Inserting (A.8) into (A.5), we can express the velocities in terms of the momenta as

$$\dot{x}^a = \frac{\alpha c}{\left[m^2c^2 + {}^{(3)}g^{-1}(\boldsymbol{p}, \boldsymbol{p})\right]^{1/2}}\,{}^{(3)}g^{ab}p_b - c\beta^a\,. \tag{A.9}$$

Using (A.8) and (A.9), the Hamiltonian corresponding to the Lagrangian (A.3) is

$$\begin{aligned} H &= p_a\dot{x}^a - L \\ &= \frac{\alpha c}{\left[m^2c^2 + {}^{(3)}g^{-1}(\boldsymbol{p}, \boldsymbol{p})\right]^{1/2}}\,{}^{(3)}g^{-1}(\boldsymbol{p}, \boldsymbol{p}) - c\beta^ap_a + \frac{m^2c^3\alpha}{\left[m^2c^2 + {}^{(3)}g^{-1}(\boldsymbol{p}, \boldsymbol{p})\right]^{1/2}} \\ &= \alpha c\left[m^2c^2 + {}^{(3)}g^{-1}(\boldsymbol{p}, \boldsymbol{p})\right]^{1/2} - c\beta^ap_a\,. \end{aligned} \tag{A.10}$$

Rewriting this in terms of the components of the spacetime metric using the relations $g^{00} = -\alpha^{-2}$, $g^{0a} = \alpha^{-2}\beta^a$, $g^{ab} = {}^{(3)}g^{ab} - \alpha^{-2}\beta^a\beta^b$, the Hamiltonian reads

$$H = \frac{1}{\sqrt{-g^{00}}}\,mc^2\left[1 + \left(g^{ab} - \frac{1}{g^{00}}g^{0a}g^{0b}\right)\frac{p_ap_b}{m^2c^2}\right]^{1/2} + \frac{c}{g^{00}}g^{0a}p_a\,. \tag{A.11}$$

B. Christoffel symbols of the Eddington–Robertson PPN metric

Here, we compute the Christoffel symbols

$$\Gamma^{\rho}_{\mu\nu} = \frac{1}{2} g^{\rho\sigma} (\partial_\mu g_{\nu\sigma} + \partial_\nu g_{\mu\sigma} - \partial_\sigma g_{\mu\nu}) \tag{B.1}$$

of the Eddington–Robertson PPN metric as given by (2.5.1), (2.5.2), keeping full track of all details of the c^{-1} expansion.

$$\begin{aligned} \Gamma^0_{00} &= \frac{1}{2} g^{00} \partial_0 g_{00} + \mathrm{O}(c^{-7}) \\ &= \frac{1}{2} \left(\frac{1}{g_{00}} + \mathrm{O}(c^{-6}) \right) \partial_0 g_{00} + \mathrm{O}(c^{-7}) \\ &= \frac{1}{2c} \partial_t \underbrace{\ln(-g_{00})}_{=2\frac{\phi}{c^2} + 2(\beta-1)\frac{\phi^2}{c^4} + \mathrm{O}(c^{-6})} + \mathrm{O}(c^{-7}) \\ &= \frac{\partial_t \phi}{c^3} + 2(\beta - 1) \frac{\phi \partial_t \phi}{c^5} + \mathrm{O}(c^{-7}) \end{aligned} \tag{B.2}$$

$$\begin{aligned} \Gamma^0_{0a} &= \frac{1}{2} g^{00} (\cancel{\partial_0 g_{0a}} + \partial_a g_{00} - \cancel{\partial_0 g_{0a}}) + \mathrm{O}(c^{-7}) \\ &= \frac{1}{2} \partial_a \ln(-g_{00}) + \mathrm{O}(c^{-6}) \\ &= \frac{\partial_a \phi}{c^2} + 2(\beta - 1) \frac{\phi \partial_a \phi}{c^4} + \mathrm{O}(c^{-6}) \end{aligned} \tag{B.3}$$

$$\begin{aligned} \Gamma^0_{ab} &= \frac{1}{2} g^{00} (\underbrace{\partial_a g_{0b} + \partial_b g_{0a}}_{=\mathrm{O}(c^{-5})} - \partial_0 g_{ab}) + \mathrm{O}(c^{-7}) \\ &= \frac{1}{2} \left(-1 + \mathrm{O}(c^{-2})\right) \frac{-1}{c} \partial_t \left(\left(1 - 2\gamma \frac{\phi}{c^2} \right) \delta_{ab} + \mathrm{O}(c^{-4}) \right) + \mathrm{O}(c^{-5}) \\ &= -\gamma \frac{\partial_t \phi}{c^3} \delta_{ab} + \mathrm{O}(c^{-5}) \end{aligned} \tag{B.4}$$

$$
\begin{aligned}
\Gamma^a_{00} &= \frac{1}{2} g^{ab} (2 \underbrace{\partial_0 g_{0b}}_{=\mathrm{O}(c^{-6})} - \partial_b g_{00}) + \mathrm{O}(c^{-7}) \\
&= \frac{1}{2} \left(\left(1 + 2\gamma \frac{\phi}{c^2} \right) \delta^{ab} + \mathrm{O}(c^{-4}) \right) \partial_b \left(1 + 2\frac{\phi}{c^2} + 2\beta \frac{\phi^2}{c^4} + \mathrm{O}(c^{-6}) \right) + \mathrm{O}(c^{-6}) \\
&= \delta^{ab} \left(\frac{\partial_b \phi}{c^2} + 2(\beta + \gamma) \frac{\phi \partial_b \phi}{c^4} \right) + \mathrm{O}(c^{-6})
\end{aligned} \tag{B.5}
$$

$$
\begin{aligned}
\Gamma^a_{0b} &= \frac{1}{2} g^{ac} (\partial_0 g_{bc} + \underbrace{\partial_b g_{0c} - \partial_c g_{0b}}_{=\mathrm{O}(c^{-5})}) + \mathrm{O}(c^{-7}) \\
&= \frac{1}{2} \left(\delta^{ac} + \mathrm{O}(c^{-2}) \right) \frac{1}{c} \partial_t \left(\left(1 - 2\gamma \frac{\phi}{c^2} \right) \delta_{bc} + \mathrm{O}(c^{-4}) \right) + \mathrm{O}(c^{-5}) \\
&= -\gamma \delta^a_b \frac{\partial_t \phi}{c^3} + \mathrm{O}(c^{-5})
\end{aligned} \tag{B.6}
$$

$$
\begin{aligned}
\Gamma^a_{bc} &= \frac{1}{2} g^{ad} (\partial_b g_{cd} + \partial_c g_{bd} - \partial_d g_{bc}) + \mathrm{O}(c^{-7}) \\
&= \frac{1}{2} \left(\delta^{ad} + \mathrm{O}(c^{-2}) \right) (-2\gamma) \left(\delta_{cd} \frac{\partial_b \phi}{c^2} + \delta_{bd} \frac{\partial_c \phi}{c^2} - \delta_{bc} \frac{\partial_d \phi}{c^2} + \mathrm{O}(c^{-4}) \right) + \mathrm{O}(c^{-7}) \\
&= -\gamma \frac{\delta^a_c \partial_b \phi + \delta^a_b \partial_c \phi - \delta_{bc} \delta^{ad} \partial_d \phi}{c^2} + \mathrm{O}(c^{-4})
\end{aligned} \tag{B.7}
$$

The last result implies $g^{bc}\Gamma^a_{bc} = \delta^{ab}\gamma\frac{\partial_b\phi}{c^2} + \mathrm{O}(c^{-4})$, in turn implying

$$
\begin{aligned}
g^{\mu\nu}\Gamma^a_{\mu\nu} &= g^{00}\Gamma^a_{00} + g^{bc}\Gamma^a_{bc} + \mathrm{O}(c^{-8}) \\
&= (-1 + \mathrm{O}(c^{-2})) \left(\delta^{ab} \frac{\partial_b \phi}{c^2} + \mathrm{O}(c^{-4}) \right) + \delta^{ab} \gamma \frac{\partial_b \phi}{c^2} + \mathrm{O}(c^{-4}) \\
&= (\gamma - 1) \delta^{ab} \frac{\partial_b \phi}{c^2} + \mathrm{O}(c^{-4}).
\end{aligned} \tag{B.8}
$$

C. Sign conventions for generators of special orthogonal groups

Here we discuss our choice of sign convention for the generators of special orthogonal groups, in particular the Lorentz group.

Let V be a finite-dimensional real vector space with a non-degenerate, symmetric bilinear form $g\colon V \times V \to \mathbb{R}$. Note that we do not assume anything about the signature of g. We introduce the 'musical isomorphism'

$$V \to V^*, v \mapsto v^\flat := g(v, \cdot) \tag{C.1}$$

induced by g.

We fix a basis $\{\mathrm{e}_a\}_a$ of V. As bases for its dual vector space V^* we distinguish its natural dual basis $\{\theta^a\}_a$, where $\theta^a(\mathrm{e}_b) = \delta^a_b$, and the ($g$-dependent) image of $\{\mathrm{e}_a\}_a$ under (C.1), which is just $\{e_a^\flat\}_a$, where $e_a^\flat = g_{ab}\theta^b$, so that $e_a^\flat(\mathrm{e}_b) = g_{ab}$. The reason for this will become clear now.

For each $a, b \in \{1, \ldots, \dim V\}$ we introduce the endomorphism

$$B_{ab} := \mathrm{e}_a \otimes \mathrm{e}_b^\flat - \mathrm{e}_b \otimes \mathrm{e}_a^\flat \in \mathrm{End}(V) \tag{C.2}$$

which satisfies

$$g(v, B_{ab}(w)) = g(v, \mathrm{e}_a) g(\mathrm{e}_b, w) - g(v, \mathrm{e}_b) g(\mathrm{e}_a, w) = -g(B_{ab}(v), w). \tag{C.3}$$

This means that B_{ab} is anti-self-adjoint with respect to g and hence that it is an element of the Lie algebra $\mathfrak{so}(V, g)$ of the Lie group $\mathrm{SO}(V, g)$ of special orthogonal transformations of (V, g):

$$B_{ab} \in \mathfrak{so}(V, g). \tag{C.4}$$

As $B_{ab} = -B_{ba}$, it is the set $\{B_{ab} : 1 \leq a < b \leq \dim V\}$ which is linearly independent and of the same dimension as $\mathfrak{so}(V, g)$. Hence this set forms a basis of $\mathfrak{so}(V, g)$ so that any $\omega \in \mathfrak{so}(V, g)$ can be uniquely written in the form

$$\omega = \sum_{1 \leq a < b \leq \dim V} \omega^{ab} B_{ab} = \frac{1}{2} \omega^{ab} B_{ab} \,, \tag{C.5}$$

where

$$\omega^{ab} = -\omega^{ba} \,. \tag{C.6}$$

This representation can easily be compared to the usual one in terms of the metric-independent basis $\{\mathrm{e}_a \otimes \theta^b : 1 \leq a, b \leq \dim V\}$ of $\mathrm{End}(V)$ in the following way: for $\omega = \omega^a{}_c\, \mathrm{e}_a \otimes \theta^c$, we have $\omega \in \mathfrak{so}(V, g)$ if and only if

$$\omega^a{}_c\, g^{cb} = -\omega^b{}_c\, g^{ca} \ . \tag{C.7}$$

It is the obvious simplicity of (C.6) as opposed to (C.7) as conditions for $\omega \in \mathrm{End}(V)$ being contained in $\mathfrak{so}(V, g) \subset \mathrm{End}(V)$ that makes it easier to work with the basis $\mathrm{e}_a \otimes \mathrm{e}_b^\flat$ of $\mathrm{End}(V)$ rather than $\mathrm{e}_a \otimes \theta^b$. Note that the components of ω with respect to the two bases considered above are connected by the equation

$$\omega^{ab} = \omega^a{}_c\, g^{cb} \ . \tag{C.8}$$

The basis elements B_{ab} satisfy the commutation relations

$$\begin{aligned} [B_{ab}, B_{cd}] &= g_{bc} B_{ad} + g_{ad} B_{bc} - g_{ac} B_{bd} - g_{bd} B_{ac} \\ &= g_{bc} B_{ad} + \text{(antisymm.)}, \end{aligned} \tag{C.9}$$

where 'antisymm.' denotes antisymmetrisation as shown in the first line of the equation.

From now on, we will assume the basis $\{\mathrm{e}_a\}_a$ to be orthonormal. For notational convenience, for $a, b \in \{1, \ldots, \dim V\}$ we define

$$\varepsilon_{ab} := g_{aa} g_{bb} = \pm 1 \tag{C.10}$$

which has the value $+1$ if $g_{aa} = g(\mathrm{e}_a, \mathrm{e}_a)$ and $g_{bb} = g(\mathrm{e}_b, \mathrm{e}_b)$ have the same sign, and -1 if they have opposite signs[1].

We now want to compute the exponential $\exp(\alpha B_{ab}) \in \mathrm{SO}(V, g)$. At first, we note that

$$\begin{aligned} (B_{ab})^2 &= -g_{bb}\, \mathrm{e}_a \otimes \mathrm{e}_a^\flat - g_{aa}\, \mathrm{e}_b \otimes \mathrm{e}_b^\flat \\ &= -\varepsilon_{ab}\, \mathrm{Pr}_{ab} \ , \end{aligned} \tag{C.11}$$

where $\mathrm{Pr}_{ab} := \mathrm{Pr}_{\mathrm{span}\{\mathrm{e}_a, \mathrm{e}_b\}}$ denotes the g-orthogonal projector onto the plane $\mathrm{span}\{\mathrm{e}_a, \mathrm{e}_b\}$

[1] Note that repeated indices on the same level, i.e. both up or both down, are not to be summed over.

in V.[2] Using this and $B_{ab} \circ \mathrm{Pr}_{ab} = B_{ab}$, the exponential series evaluates to

$$\begin{aligned}
\exp(\alpha B_{ab}) &= (\mathrm{id}_V - \mathrm{Pr}_{ab}) + \sum_{k=0}^{\infty} \frac{1}{(2k)!}\, \alpha^{2k} (-\varepsilon_{ab})^k\, \mathrm{Pr}_{ab} \\
&\quad + \sum_{k=0}^{\infty} \frac{1}{(2k+1)!}\, \alpha^{2k+1} (-\varepsilon_{ab})^k\, B_{ab} \circ \mathrm{Pr}_{ab} \\
&= (\mathrm{id}_V - \mathrm{Pr}_{ab}) + \left\{ \begin{matrix} \cos(\alpha)\, \mathrm{id}_V + \sin(\alpha)\, B_{ab}\,, & \varepsilon_{ab} = +1 \\ \cosh(\alpha)\, \mathrm{id}_V + \sinh(\alpha)\, B_{ab}\,, & \varepsilon_{ab} = -1 \end{matrix} \right\} \circ \mathrm{Pr}_{ab}\,. \qquad \text{(C.12)}
\end{aligned}$$

Geometrically, this transformation is either a rotation by angle α (for $\varepsilon_{ab} = +1$) or a boost by rapidity α (for $\varepsilon_{ab} = -1$) in the plane $\mathrm{span}\{\mathrm{e}_a, \mathrm{e}_b\}$. The direction of the transformation depends on the signs of g_{aa}, g_{bb}:

- $\varepsilon_{ab} = +1$:
  - (i) $g_{aa} = g_{bb} = +1$: We have $B_{ab}(\mathrm{e}_a) = -\mathrm{e}_b, B_{ab}(\mathrm{e}_b) = \mathrm{e}_a$. Thus, $\exp(\alpha B_{ab})$ is a rotation by α *from* e_b *towards* e_a.
  - (ii) $g_{aa} = g_{bb} = -1$: We have $B_{ab}(\mathrm{e}_a) = \mathrm{e}_b, B_{ab}(\mathrm{e}_b) = -\mathrm{e}_a$. Thus, $\exp(\alpha B_{ab})$ is a rotation by α *from* e_a *towards* e_b.
- $\varepsilon_{ab} = -1$:
  - (i) $g_{aa} = +1, g_{bb} = -1$: We have $B_{ab}(\mathrm{e}_a) = -\mathrm{e}_b, B_{ab}(\mathrm{e}_b) = -\mathrm{e}_a$. Thus, $\exp(\alpha B_{ab})$ is a boost by α *'away' from* $\mathrm{e}_a + \mathrm{e}_b$.
  - (ii) $g_{aa} = -1, g_{bb} = +1$: We have $B_{ab}(\mathrm{e}_a) = \mathrm{e}_b, B_{ab}(\mathrm{e}_b) = \mathrm{e}_a$. Thus, $\exp(\alpha B_{ab})$ is a boost by α *'towards'* $\mathrm{e}_a + \mathrm{e}_b$.

Now we will apply the preceding considerations to the case of (the 'difference' vector space of) Minkowski spacetime, where for now *we leave open the signature convention for the metric* (either $(+---)$ or $(-+++)$). We work with respect to a positively oriented orthonormal basis $\{\mathrm{e}_\mu\}_{\mu=0,\dots,3}$ where e_0 is timelike. Latin indices will denote spacelike directions.

[2]In the general case of two linearly independent vectors $v, w \in V$, not necessarily orthonormal, the orthogonal projector is given by

$$\mathrm{Pr}_{\mathrm{span}(v,w)} = \frac{1}{g(v,v)g(w,w) - (g(v,w))^2} \Big[g(w,w)\; v \otimes v^\flat + g(v,v)\; w \otimes w^\flat - g(v,w)\; (v \otimes w^\flat + w \otimes v^\flat) \Big]\,,$$

implying

$$\begin{aligned}
(v \otimes w^\flat - w \otimes v^\flat)^2 &= -g(w,w)\; v \otimes v^\flat - g(v,v)\; w \otimes w^\flat + g(v,w)\; (v \otimes w^\flat + w \otimes v^\flat) \\
&= -\Big[g(v,v)g(w,w) - (g(v,w))^2 \Big]\, \mathrm{Pr}_{\mathrm{span}(v,w)}.
\end{aligned}$$

In the case of 'mostly minus' signature $(+---)$, B_{ab} generates rotations from e_a towards e_b and B_{a0} generates boosts (with respect to e_0) in direction of e_a. In the case of 'mostly plus' signature $(-+++)$, $B_{ba} = -B_{ab}$ generates rotations from e_a towards e_b and $B_{0a} = -B_{a0}$ generates boosts (with respect to e_0) in direction of e_a.

Thus, since we want to use the notation J_{ab} for the spacelike rotational generator generating rotations from e_a towards e_b, we have to set

$$J_{\mu\nu} = \begin{cases} B_{\mu\nu} & \text{for } (+---) \text{ signature,} \\ -B_{\mu\nu} & \text{for } (-+++) \text{ signature} \end{cases} \tag{C.13}$$

for the Lorentz generators. Adopting this convention, boosts in direction of e_a are then generated by J_{a0}. The commutation relations for the $J_{\mu\nu}$ are

$$[J_{\mu\nu}, J_{\rho\sigma}] = \begin{cases} \eta_{\mu\sigma} J_{\nu\rho} + (\text{antisymm.}) & \text{for } (+---) \text{ signature,} \\ \eta_{\mu\rho} J_{\nu\sigma} + (\text{antisymm.}) & \text{for } (-+++) \text{ signature,} \end{cases} \tag{C.14}$$

and general Lorentz algebra elements $\omega \in \mathrm{Lie}(\mathcal{L})$ can be written as

$$\omega = \pm\frac{1}{2}\omega^{\mu\nu} J_{\mu\nu} \text{ with } \omega^{\mu\nu} = \omega^{\mu}{}_{\rho}\, \eta^{\rho\nu} \tag{C.15}$$

in terms of their components $\omega^{\mu}{}_{\rho}$ as endomorphisms, where the upper/lower sign holds for $(+---)/(-+++)$ signature.

D. Notes on the adjoint representation

Here we wish to make a few remarks and collect a few formulae concerning the adjoint and co-adjoint representation of the general linear group of a vector space V.

In the defining representation on V, an element $\Lambda \in \mathrm{GL}(V)$ is given in terms of the basis $\{e_a\}_a$ by the coefficients $\Lambda^a{}_b$, where

$$\Lambda\, e_a = \Lambda^b{}_a\, e_b \ . \tag{D.1}$$

This defines a left action of $\mathrm{GL}(V)$ on V. The corresponding left action of $\mathrm{GL}(V)$ on the dual space V^* is given by the inverse-transposed, i.e. $\mathrm{GL}(V) \times V^* \to V^*$, $(\Lambda, \alpha) \mapsto (\Lambda^{-1})^\top \alpha := \alpha \circ \Lambda^{-1}$. For the basis $\{\theta^a\}_a$ of V^* dual to the basis $\{e_a\}_a$ this means

$$\theta^a \circ \Lambda^{-1} = (\Lambda^{-1})^a{}_b\, \theta^b \ . \tag{D.2}$$

In contrast, for the basis $\{e^\flat_a\}_a$ of V^*, this reads in general

$$e^\flat_b \circ \Lambda^{-1} = g^{ac} g_{bd} (\Lambda^{-1})^d{}_c\, e^\flat_a \ , \tag{D.3}$$

which for isometries $\Lambda \in \mathrm{O}(V, g)$ simply becomes

$$e^\flat_b \circ \Lambda^{-1} = \Lambda^a{}_b\, e^\flat_a \ . \tag{D.4}$$

The adjoint representation of $\mathrm{GL}(V)$ on $\mathrm{End}(V) \cong V \otimes V^*$ or any Lie subalgebra of $\mathrm{End}(V)$ is by conjugation, which for our basis (C.2) implies, using (D.1) and (D.4),

$$\mathrm{Ad}_\Lambda B_{ab} = \Lambda \circ B_{ab} \circ \Lambda^{-1} = \Lambda^c{}_a \Lambda^d{}_b\, B_{cd} \quad \text{for } \Lambda \in \mathrm{O}(V, g). \tag{D.5}$$

The adjoint representation of the inhomogeneous group $\mathrm{GL}(V) \ltimes V$ on its Lie algebra $\mathrm{End}(V) \oplus V$ is given by, for any $X \in \mathrm{End}(V)$ and $y \in V$,

$$\mathrm{Ad}_{(\Lambda, a)}(X, y) = \Big(\Lambda \circ X \circ \Lambda^{-1}, \Lambda y - (\Lambda \circ X \circ \Lambda^{-1}) a\Big) \, . \tag{D.6}$$

In the main text we will use this formula for (Λ, a) being replaced by its inverse $(\Lambda, a)^{-1} = (\Lambda^{-1}, -\Lambda^{-1}a)$:

$$\mathrm{Ad}_{(\Lambda,a)^{-1}}(X, y) = \Big(\Lambda^{-1} \circ X \circ \Lambda, \Lambda^{-1}y + (\Lambda^{-1} \circ X)a\Big) \tag{D.7}$$

Applied to the basis vectors separately, i.e. to $(X, y) = (0, \mathrm{e}_b)$ and $(X, y) = (B_{bc}, 0)$, for $\Lambda \in \mathrm{O}(V, g)$ we get

$$\mathrm{Ad}_{(\Lambda,a)^{-1}}(0, \mathrm{e}_b) \;= \Big(0, (\Lambda^{-1})^c{}_b\, \mathrm{e}_c\Big)\,, \tag{D.8a}$$

$$\mathrm{Ad}_{(\Lambda,a)^{-1}}(B_{bc}, 0) = \Big((\Lambda^{-1})^d{}_b(\Lambda^{-1})^e{}_c\, B_{de}, -a_b(\Lambda^{-1})^d{}_c\, \mathrm{e}_d + a_c(\Lambda^{-1})^d{}_b\, \mathrm{e}_d\Big) \tag{D.8b}$$

where $a_b := \mathrm{e}_b^\flat(a) = g_{bc}a^c$ in the second equation. From these equations we immediately deduce (5.2.20) in the case of four spacetime dimensions (greek indices) and signature mostly plus, in which case $J_{\mu\nu} = -B_{\mu\nu}$ according to (C.13).

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Scholarships

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