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

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We extend the systematic calculation of an approximately relativistic Hamiltonian for center of mass and internal dynamics of an electromagnetically bound two-particle system by Sonnleitner and Barnett [Phys. Rev. A **98**, 042106 (2018)] to the case including a weak post-Newtonian gravitational background field, described by the Eddington-Robertson parametrized post-Newtonian metric. Starting from a proper relativistic description of the situation, this approach allows us to systematically derive the coupling of the model system to gravity, instead of "guessing" it by means of classical notions of relativistic effects. We embed this technical result into a critical discussion concerning the problem of implementing and interpreting general couplings to the gravitational field and the connected problem of how to properly address the question concerning the validity of the Equivalence Principle in Quantum Mechanics.

I. INTRODUCTION

Experiments in quantum optics and matter-wave interferometry have now reached a degree of precision that covers "new" relativistic corrections that were hitherto not considered in such settings. In particular, this includes couplings between "internal" and "center of mass" degrees of freedom of composite systems, which have no Newtonian analog. Hence, such experiments require proper relativistic treatments for their theoretical descriptions. Quite generally, such descriptions are often restricted to more or less *ad hoc* addition of "effects" known from classical physics, like velocity-dependent masses, second-order Doppler shifts, second-order aberrations, redshifted energies, and time dilations due to relative velocities and/or gravitational potentials. Such approaches are conceptually dangerous for a number of reasons. Neither do they guarantee completeness and independence, nor do they need to apply in nonclassical situations where quantum properties dominate the dynamics. Such "derivations" often obscure the proper physical interpretation of relativistic corrections and, consequently, potentially misguide physical conclusions drawn form their observation.

An example of this sort has recently been discussed in the careful and lucid analysis by Sonnleitner and Barnett [1], who pointed out that certain terms that show up in computations of the interaction of moving atoms with light, and which from a nonrelativistic[1] point of view appear to be some kind

of "friction" (of a non-immediately obvious physical origin, hence one may be tempted to call them "anomalous"), are actually nothing but a straightforward consequence of Special Relativity. In fact, there is nothing to be surprised about once the calculation is done, and the results are interpreted, in a proper relativistic framework. This was done approximately in Ref. [1] for the gravity-free case, by systematically deriving an "approximately relativistic" Hamiltonian describing the atom. It is the purpose of our paper to extend this so as to also include gravity approximately. As emphasized above, this generalization serves not only a point of principal interest that deserves clarification, but is also of immediate practical interest, not only in the obvious realm of quantum optics experiments regarding the detection of gravitational waves, but also in atom interferometry; see, e.g., Refs. [2–8]. A calculation using methods very similar to those of Ref. [1] including external gravitational fields was performed by Marzlin already in 1995 [9]; but unlike Sonnleitner and Barnett in Ref. [1] or our calculation in this work, Marzlin did not perform a full first-order post-Newtonian expansion and instead focused on the electric dipole coupling only.

What is generally needed is a consistent post-Newtonian approximation scheme in which the transition from Galilei invariant to Poincaré invariant (Special Relativity) and further to diffeomorphism invariant (General Relativity) laws can be systematically derived in a step-by-step algorithmic fashion. Such a scheme must be fundamentally rooted in a principle that contains all the information of how matter couples to gravity.

For classical matter, described in terms of dynamical laws compatible with the requirements of Special Relativity, such a

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[1]As a matter of principle, we would like to avoid the common but misleading adjective "nonrelativistic" 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 physical relativity principle that distinguishes both cases. Rather, their difference lies in the way that principle is implemented. Since

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we cannot entirely escape traditionally established nomenclature without undue complications in expression, we will continue to use the term "nonrelativistic" in the sense just explained and think of it as always being put between (invisible) inverted commas.

principle is known in form of the "minimal coupling scheme." According to this scheme, the Minkowski metric of Special Relativity is to be replaced by the more general Lorentzian metric of spacetime and all partial derivatives (or more precisely: Levi-Civita covariant derivatives with respect to the Minkowski metric) are to be replaced with the Levi-Civita covariant derivatives with respect to the general spacetime metric. This scheme is based on Einstein's Equivalence Principle, whose core statement is that gravity can be encoded in the geometry of spacetime *that is common to all matter components*. We stress that this is the important point encoding the *universality* of gravitational interaction: that any matter component, may it be light, neutrinos, or other elementary particles with or without mass, spin, charge, or other features, or may it be a macroscopic body, like a football or a planet, all of them will couple to gravity in a way that only depends on one and the same geometry of spacetime; compare Ref. [10].

The problem we face in quantum physics as regards its coupling to gravitational fields is that the minimal coupling scheme has no straightforward generalization to Galilei invariant Quantum Mechanics, for the obvious reason that the latter is incompatible with the requirements of Special Relativity. As is well known, enforcing Poincaré symmetry upon Quantum Mechanics eventually leads to the framework of Poincaré invariant Quantum Field Theory, often referred to as "Relativistic Quantum Field Theory" (RQFT), whose mathematical structure and physical interpretation is far more complex than that of ordinary nonrelativistic Quantum Mechanics. As a matter of principle, a post-Newtonian expansion should therefore start from RQFT.

However, if one is merely interested in leading order "relativistic corrections" below the threshold of pair production for any of the massive particles involved, a simpler method is to first put the *classical* system in a fixed particle sector into Poincaré invariant form, then apply the minimal coupling scheme on the classical level, and finally apply suitable rules for quantization, like the canonical ones. This is the procedure we will follow in this paper. It is computationally and conceptually much cheaper than a proper quantum field theoretic treatment and is *a priori* limited to sectors of fixed numbers in each massive particle species (hence it would not make sense to carry the computation of "relativistic corrections" further than to the lowest lying particle-production threshold). In fact, the corrections we are after are far from those thresholds and may be safely derived from a systematic post-Newtonian expansion on the classical level.

It is the underlying systematics of producing "relativistic corrections" that, in our opinion, distinguishes our approach from others, like, e.g., Refs. [3–8]. These latter attempts make use in an essential way of 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. More precisely, the state of the total system (the atom) is assumed to unambiguously define a worldline, say, for the center of mass, which can also be assigned a length that is then identified with the proper time (up to division by a factor of c). This implies that (1) the overall pure state of the system separates into the tensor product of a pure state for the center of mass with a pure state for the relative degrees of freedom, and that (2) the state for the center of mass is

of semiclassical nature, so as to unambiguously determine a piecewise smooth (C^1) worldline.[2] It may well be that these *a priori* restrictions can be justified in specific applications within quantum optics and atom interferometry. However, here we wish to promote the view that the theoretical problem of formulating a consistent post-Newtonian coupling scheme should be solved *independently* of such restrictions.

In addition, phrasing relativistic corrections in terms of classical notions like "proper times," "redshifts," and the like bears the danger of losing control over aspects of completeness and possible redundancies. To be sure, these classical "effects" will appear as consequences from the general scheme, if applied to the specific situation that allows such vocabulary. But they should not be mistaken for the relativistic corrections proper, which derive from the spacetime geometry as a whole that enters the quantum dynamical laws at a fundamental level. Similar remarks apply in connection with attempts to formulate the Equivalence Principle in Quantum Mechanics. Since we consider this to be an important and directly related issue, which also bears the danger of misconceptions, we will devote an extra section to its discussion at the end of this paper.

Problems of this sort were avoided by Sonnleitner and Barnett [1] by the means of basing their whole calculation on a proper relativistic treatment of the situation (an atom interacting with an external electromagnetic field). 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": The "center of mass" part of the final Hamiltonian has the form of a single-particle kinetic Hamiltonian, where the role 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 consituent particles and the internal atomic energy divided by c^2. Thus, the computation in Ref. [1] 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 in this paper, 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 center of mass dynamics. Our essential result in that respect is expressed by Eqs. (5.5) to (5.8). 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.

Logical structure of this paper

In Sec. II we set up the background for our calculations: after describing the physical system under consideration, we

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[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.

will give an overview over the method of computation in Ref. [1]. Then we will discuss the geometric structures necessary to perform a post-Newtonian limit and to describe weak gravitational fields.

In the following, we will compute in detail the "gravitational corrections" to the calculation by Sonnleitner and Barnett [1] arising from the presence of the gravitational field. Section III 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 Sec. IV 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 Sec. V A, by repeating the calculation from Sec. III while including the "gravitational corrections" to electromagnetism obtained in Sec. IV. The resulting Hamiltonian will then be interpreted in terms of the physical spacetime metric and compared to earlier results in the remainder of Sec. V.

In Sec. VI we will critically discuss attempts of formulating the Equivalence Principle in Quantum Mechanics, before concluding in Sec. VII with a brief summary of our paper.

In Secs. III and V A, we will very closely follow the calculation from and presentation in Ref. [1]. For the reader's convenience, we have reproduced all formulas from Ref. [1] that are used in our calculation in the Appendix. We use the original numbering, prepended with "A[1].," so, for example, (A[1].25f) refers to Eq. (25f) of Ref. [1]. As some of the equations from Ref. [1] contain minor errors (mostly sign errors), we give the corrected versions in the Appendix. The corresponding equation numbers are marked with an asterisk, e.g., (A[1].12*).

II. 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 $\mathbf{r}_1, \mathbf{r}_2$. For simplicity we assume the charges to be equal and opposite, $e_2 = -e_1 =: e$. 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, that we will also take into account. It is the inclusion of the latter that we wish to discuss in this paper and that extends previous studies [1].

A. External electromagnetic fields: The work of Sonnleitner and Barnett

In Ref. [1] 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 [11,12] 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 nonrelativistic (i.e., Galilei invariant) setting of ordinary Quantum Mechanics. Their correct conclusion in Ref. [1] was that this confusion can be altogether avoided by replacing this "hotchpotch" (their wording; see the last line on p. 042106-9 of Ref. [1]) of symmetry concepts by a systematic post-Newtonian derivation starting from a common, manifestly Poincaré symmetric description.

As our development will closely follow theirs, let us describe the strategy of Ref. [1] in more detail. They start with the classical Poincaré invariant Lagrangian function describing the situation, where the kinetic terms of the two particles are expanded to post-Newtonian order. This Lagrangian includes the electromagnetic fields generated by the particles themselves as lowest-order solutions of the Maxwell equations, thus eliminating the "internal" field degrees of freedom.

This classical Lagrangian (the sum of the famous Darwin Lagrangian [13] and the external field Lagrangian) is then Legendre transformed and canonically quantized to obtain a quantum Hamiltonian in what they call the "minimal coupling form." They then perform a Power-Zienau-Woolley (PZW) unitary transformation [14–16] together with a multipolar expansion of the external field in order to transform the Hamiltonian into a so-called "multipolar form."

Then, introducing Newtonian center of mass and relative coordinates $\mathbf{R}, \mathbf{r}$, and the corresponding canonical momenta $\mathbf{P}, \mathbf{p_r}$, they arrive at what they call the center of mass Hamiltonian. This can be separated into parts describing the central motion of the atom, the internal atomic motion, the external electromagnetic field, and its interaction with the atom. However, this Hamiltonian also contains cross terms coupling the relative degrees of freedom to the central momentum $\mathbf{P}$. In order to eliminate this coupling, they perform a final canonical transformation to new coordinates $\mathbf{Q}, \mathbf{q}$ and momenta $\mathbf{P}, \mathbf{p}$.

B. Including weak external gravitational fields

As already stated above, our contribution in this paper will consist in generalizing the calculation of Ref. [1] to the case of the atom being situated in a weak external gravitational field in addition to the electromagnetic field already considered in Ref. [1]. Our aim is to likewise obtain an "approximately relativistic," i.e., first-order post-Newtonian, Hamiltonian describing this situation.

Conceptually speaking, this generalization is not entirely obvious for the following reason: The addition of gravitational fields will, according to General Relativity, result in a changed geometry of spacetime and, consequently, in the loss of some or all spacetime symmetries and their associated conservation laws. In particular, Poincaré symmetry will be lost and there is no obvious way to implement the post-Newtonian expansion employed in Ref. [1]. In fact, the concept of a "post-Newtonian expansion" in an arbitrary spacetime simply does not exist without the explicit introduction of certain background structures that give meaning to notions like "weak" gravitational fields and "slow" velocities. To cut a long story short, such necessary background structures will

in our case be (1) the Poincaré symmetric Minkowski metric η on spacetime M and (2) a preferred inertial reference frame in Minkowski space (M, η), mathematically represented by a timelike vector field u which is geodesic for η.

That the gravitational field be weak then means that the physical spacetime metric g deviates only little from the Minkowski metric η. More precisely this means in our case that quadratic and higher orders of the difference $h := g - \eta$ and its derivatives can be neglected. That velocities be slow means that the velocity v of each particle relative to the preferred frame is small to c, so that terms in v/c of higher order than the second can be neglected.

We stress that all the structures introduced and all the conditions of "weakness" and "slowness" mentioned are totally independent of coordinates that we may choose to parametrize spacetime. 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, so-called inertial coordinates $\{x^0, x^1, x^2, x^3\}$ in Minkowski space (M, η), such that $x^0 = ct$, $u = \partial/\partial t$, and $\eta = \eta_{\mu\nu} dx^\mu \otimes dx^\nu$ with $(\eta_{\mu\nu}) = \mathrm{diag}(-1, 1, 1, 1)$. In the same coordinate system, the components of the physical spacetime metric $g = g_{\mu\nu} dx^\mu \otimes dx^\nu$ that we consider here are then given by

$$
(g_{\mu\nu}) = \begin{pmatrix} -1 - 2\frac{\phi}{c^2} - 2\beta\frac{\phi^2}{c^4} + O(c^{-6}) & O(c^{-5}) \\ O(c^{-5}) & \left(1 - 2\gamma\frac{\phi}{c^2}\right)\mathbb{1} + O(c^{-4}) \end{pmatrix}, \tag{2.1}
$$

where ϕ is a scalar function on spacetime that may be seen as the analog of the Newtonian gravitational potential in this approximation scheme. The weakness of the gravitational field is expressed in components by $|h_{\mu\nu}| = |g_{\mu\nu} - \eta_{\mu\nu}| \ll 1$. Using (2.1) this is equivalent to the smallness of the Newtonian potential as compared to c^2, that is $\phi/c^2 \ll 1$.

The metric (2.1) also contains two dimensionless parameters β and γ, the so-called "Eddington-Robertson parameters," which we introduced in order to account for possible deviations from General Relativity. General Relativity corresponds to the values $\beta = \gamma = 1$, in which case the metric (2.1) solves the field equations of General Relativity approximately in a $1/c$-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; see, e.g.,

Ref. [17]. Following standard terminology, we shall refer to (2.1) as the "PPN metric" (parametrized post-Newtonian). The explicit inclusion of β and γ in our formalism allows us to track the consequences of post-Newtonian corrections in the spatial and the temporal part of the metric separately. This also opens the possibility to apply our results to potential future quantum tests of General Relativity itself, which are outside the scope of this paper.

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 $^{(3)}g^{-1}$.

Later we will also need the inverse metric to g, the components of which in the specified coordinate system are simply obtained by inverting the matrix (2.1):

$$
(g^{\mu\nu}) = \begin{pmatrix} -1 + 2\frac{\phi}{c^2} + (2\beta - 4)\frac{\phi^2}{c^4} + O(c^{-6}) & O(c^{-5}) \\ O(c^{-5}) & \left(1 + 2\gamma\frac{\phi}{c^2}\right)\mathbb{1} + O(c^{-4}) \end{pmatrix}. \tag{2.2}
$$

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 nonlocal in time, spoiling the application of the Hamiltonian formalism.

C. Geometric structures, notation, and conventions

The chosen background structures that allow us to define the approximation scheme (according to "slow" and "weak") are also employed in developing our calculation in parallel with that in Ref. [1]. More precisely, we use the background Minkowski metric η and the preferred timelike vector field

u to decompose spacetime into time (integral lines of u) and space (hyperplanes η-perpendicular to u), and to endow space with a flat Riemannian metric (the restriction of η to the hyperplanes). With that structure "space" just becomes ordinary flat Euclidean space. We are indeed free to use this "flat" structure to perform all our computations, the benefit being the aimed-for direct comparison with Ref. [1]. However, once the results of the computations 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 it is precisely this reinterpretation of the formulas obtained that lends them good physical meaning.

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- 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) and the spatial metric its usual Euclidean form with components of the metric tensor given by $(\delta_{ab}) = \mathrm{diag}(1, 1, 1)$ and its inverse $(\delta^{ab}) = \mathrm{diag}(1, 1, 1)$.

We will often employ a "three-vector" notation, where the three-tuple of spatial components of some quantity will be denoted by an upright, boldface letter: for example, $\mathbf{r}_1$ is the "vector" of spatial coordinates of the first particle. When using this notation, a dot between two such "vectors" will denote the *component-wise* "Euclidean scalar product":

$$\mathbf{v} \cdot \mathbf{w} := \delta_{ab} v^a w^b = \sum_{a=1}^{3} v^a w^a, \tag{2.3}$$

and a cross multiplication symbol will denote the *component-wise* vector product,

$$(\mathbf{v} \times \mathbf{w})^a := \delta^{an} \varepsilon_{nbc} v^b w^c, \tag{2.4}$$

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

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

$$\boldsymbol{\nabla} = (\partial_1, \partial_2, \partial_3), \tag{2.5}$$

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 shorthand notation, for example, writing

$$(\boldsymbol{\nabla} \times \mathbf{A})^a = \varepsilon^{abc} \partial_b A_c \tag{2.6}$$

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

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, 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. This fact is very important to keep in mind if it comes to the task of interpreting the results of computations. For example, these results will contain geometric operations, like scalar products, which my be taken using either of the metric structures provided by the formalism. What may then appear as a more or less complicated gravitational correction to the flat space result will then, 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., Refs.. [9,18]. For us, too, they will once more turn out to be relevant in connection with the total Hamiltonian in Sec. V A and the ensuing discussion in Sec. V C. 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 Ref. [1],

but then we shall reinterpret the results in terms of the proper physical metric g in order to reveal their naturalness.

III. 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 Ref. [1] to obtain a quantum Hamiltonian in center of mass coordinates.

A. The classical Hamiltonian

For a single free point particle with mass m and position $\mathbf{x}$, the classical kinetic Lagrangian (parametrizing the worldline by coordinate time) in our metric (2.1) reads

$$\begin{aligned} L_{\mathrm{point}} &= -mc^2 \sqrt{-g_{\mu\nu} \dot{x}^\mu \dot{x}^\nu / c^2} \\ &= \frac{m\dot{\mathbf{x}}^2}{2}\left(1 + \frac{\dot{\mathbf{x}}^2}{4c^2}\right) - mc^2 - m\phi\left[1 + (2\beta - 1)\frac{\phi}{2c^2}\right] \\ &\quad - \frac{2\gamma + 1}{2}\frac{m\phi}{c^2}\dot{\mathbf{x}}^2 + O(c^{-4}). \end{aligned} \tag{3.1}$$

Now considering our two-particle system, the kinetic terms for the particles in gravity are given as the sum of two terms as in (3.1). These lowest-order "gravitationally corrected" kinetic terms we include into the classical Lagrangian from (A[1].4),[3] which described two particles interacting with an electromagnetic field in the *absence* of gravity.

Eliminating the internal electromagnetic fields literally as in Ref. [1], we arrive at the post-Newtonian classical Lagrangian,

$$\begin{aligned} L_{\mathrm{new}} &= L - m_1\phi(\mathbf{r}_1) - m_2\phi(\mathbf{r}_2) \\ &\quad - \frac{2\gamma + 1}{2}\frac{m_1\phi(\mathbf{r}_1)}{c^2}\dot{\mathbf{r}}_1^2 - \frac{2\gamma + 1}{2}\frac{m_2\phi(\mathbf{r}_2)}{c^2}\dot{\mathbf{r}}_2^2 \\ &\quad - (2\beta - 1)\frac{m_1\phi(\mathbf{r}_1)^2}{2c^2} - (2\beta - 1)\frac{m_2\phi(\mathbf{r}_2)^2}{2c^2}, \end{aligned} \tag{3.2}$$

describing our electromagnetically bound two-particle system and the external electromagnetic field. Here L is the final classical Lagrangian from (A[1].8) and (A[1].9).

Legendre transforming this with respect to the particle velocities $\dot{\mathbf{r}}_i$ and the time derivative $\partial_t \mathbf{A}^\perp$ of the electromagnetic vector potential, we obtain the total classical Hamiltonian

$$\begin{aligned} H_{\mathrm{new}} &= H + m_1\phi(\mathbf{r}_1) + m_2\phi(\mathbf{r}_2) \\ &\quad + \frac{2\gamma + 1}{2m_1 c^2}\phi(\mathbf{r}_1)\bar{\mathbf{p}}_1^2 + \frac{2\gamma + 1}{2m_2 c^2}\phi(\mathbf{r}_2)\bar{\mathbf{p}}_2^2 \\ &\quad + (2\beta - 1)\frac{m_1\phi(\mathbf{r}_1)^2}{2c^2} + (2\beta - 1)\frac{m_2\phi(\mathbf{r}_2)^2}{2c^2}. \end{aligned} \tag{3.3}$$

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[3]We remind the reader that all the equations from Ref. [1] that we refer to explicitly are reproduced in the Appendix.

Here H is the classical Hamiltonian from (A[1].12*) and $\bar{\mathbf{p}}_i = \mathbf{p}_i - e_i \mathbf{A}^\perp(\mathbf{r}_i)$ is the kinetic momentum. Note that we dropped all terms that go beyond our order of approximation.

B. Canonical quantization and PZW transformation to a multipolar Hamiltonian

Now, we canonically quantise this Hamiltonian and perform the PZW transformation and electric dipole approximation used in [1] to arrive at the "multipolar" Hamiltonian from (A[1].23*). Neglecting terms of the form $\frac{\mathbf{p}_i \cdot [\mathbf{d} \times \mathbf{B}(\mathbf{R})]}{m_i m_j c^2}$ as in (A[1].22), in our gravitational correction terms from (3.3) these transformations amount just to the replacement $\bar{\mathbf{p}}_i \rightarrow \mathbf{p}_i$ (compare the Appendix from (A[1].14*) to (A[1].21*)). Hence the multipolar Hamiltonian including the gravitational correction terms is

$$
\begin{aligned}
H_{[\text{mult}],\text{new}} = {} & H_{[\text{mult}]} + m_1 \phi(\mathbf{r}_1) + m_2 \phi(\mathbf{r}_2) \\
& + \frac{2\gamma + 1}{2m_1 c^2} \mathbf{p}_1 \cdot \phi(\mathbf{r}_1)\mathbf{p}_1 + \frac{2\gamma + 1}{2m_2 c^2} \mathbf{p}_2 \cdot \phi(\mathbf{r}_2)\mathbf{p}_2 \\
& + (2\beta - 1)\frac{m_1 \phi(\mathbf{r}_1)^2}{2c^2} + (2\beta - 1)\frac{m_2 \phi(\mathbf{r}_2)^2}{2c^2},
\end{aligned}
\tag{3.4}
$$

where $H_{[\text{mult}]}$ is the multipolar Hamiltonian from (A[1].23*).

Now that we are on the quantum level, we had to choose a symmetrized operator ordering for the $\mathbf{p}^2\phi$ terms. We chose an ordering of the form $\mathbf{p} \cdot \phi\mathbf{p}$ since that is an "obvious" choice, which also results if a WKB-like expansion of the Klein-Gordon equation is used for the description of single quantum particles in an Eddington-Robertson PPN metric [19], when one neglects terms involving $\Delta\phi$ (which vanishes outside the matter generating the Newtonian potential ϕ).

C. Introduction of center of mass variables

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

$$
\mathbf{R} = \frac{m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2}{M}, \quad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2,
\tag{3.5}
$$

$$
\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2, \quad \mathbf{p}_{1,2} = \frac{m_{1,2}}{M}\mathbf{P} \pm \mathbf{p}_{\mathbf{r}},
\tag{3.6}
$$

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

$$
\begin{aligned}
& \mathbf{p}_{1,2} \cdot \phi(\mathbf{r}_{1,2})\mathbf{p}_{1,2} \\
& = \left(\frac{m_{1,2}}{M}\mathbf{P} \pm \mathbf{p}_{\mathbf{r}}\right) \cdot \phi(\mathbf{r}_{1,2})\left(\frac{m_{1,2}}{M}\mathbf{P} \pm \mathbf{p}_{\mathbf{r}}\right) \\
& = \frac{m_{1,2}^2}{M^2}\mathbf{P} \cdot \phi(\mathbf{r}_{1,2})\mathbf{P} \pm \frac{m_{1,2}}{M}[\mathbf{P} \cdot \phi(\mathbf{r}_{1,2})\mathbf{p}_{\mathbf{r}} + \text{H.c.}] \\
& \quad + \mathbf{p}_{\mathbf{r}} \cdot \phi(\mathbf{r}_{1,2})\mathbf{p}_{\mathbf{r}}
\end{aligned}
\tag{3.7}
$$

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

$$
\begin{aligned}
& \frac{1}{m_1}\phi(\mathbf{r}_1) + \frac{1}{m_2}\phi(\mathbf{r}_2) \\
& = \left(\frac{1}{m_1} + \frac{1}{m_2}\right)\phi(\mathbf{R}) + \frac{1}{M}\left(\frac{m_2}{m_1} - \frac{m_1}{m_2}\right)\mathbf{r} \cdot \nabla\phi(\mathbf{R}) \\
& = \frac{1}{\mu}\phi(\mathbf{R}) - \frac{m_1 - m_2}{m_1 m_2}\mathbf{r} \cdot \nabla\phi(\mathbf{R}),
\end{aligned}
\tag{3.8}
$$

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

$$
\begin{aligned}
H_{[\text{com}],\text{new}} = {} & H_{[\text{com}]} + M\phi(\mathbf{R}) + (2\beta - 1)\frac{M\phi(\mathbf{R})^2}{2c^2} \\
& + \frac{2\gamma + 1}{2Mc^2}\mathbf{P} \cdot \phi(\mathbf{R})\mathbf{P} + \frac{2\gamma + 1}{2\mu c^2}\mathbf{p}_{\mathbf{r}}^2\phi(\mathbf{R}) \\
& + \frac{2\gamma + 1}{2Mc^2}\{\mathbf{P} \cdot [\mathbf{r} \cdot \nabla\phi(\mathbf{R})]\mathbf{p}_{\mathbf{r}} + \text{H.c.}\} \\
& - \frac{2\gamma + 1}{2c^2}\frac{m_1 - m_2}{m_1 m_2}\mathbf{p}_{\mathbf{r}} \cdot [\mathbf{r} \cdot \nabla\phi(\mathbf{R})]\mathbf{p}_{\mathbf{r}}, \quad (3.9)
\end{aligned}
$$

where $H_{[\text{com}]}$ is the center of mass Hamiltonian from (A[1].25*).

This can, as in [1], be brought into the form

$$
H_{[\text{com}],\text{new}} = H_{\text{C,new}} + H_{\text{A,new}} + H_{\text{AL}} + H_{\text{L}} + H_{\text{X,new}}, \tag{3.10}
$$

where

$$
\begin{aligned}
H_{\text{C,new}} = {} & H_{\text{C}} + \frac{2\gamma + 1}{2Mc^2}\mathbf{P} \cdot \phi(\mathbf{R})\mathbf{P} \\
& + \left(M + \frac{\mathbf{p}_{\mathbf{r}}^2}{2\mu c^2}\right)\phi(\mathbf{R}) + (2\beta - 1)\frac{M\phi(\mathbf{R})^2}{2c^2}
\end{aligned}
\tag{3.11}
$$

describes the dynamics of the center of mass and

$$
\begin{aligned}
H_{\text{A,new}} = {} & H_{\text{A}} + 2\gamma\frac{\phi(\mathbf{R})}{c^2}\frac{\mathbf{p}_{\mathbf{r}}^2}{2\mu} \\
& - \frac{2\gamma + 1}{2c^2}\frac{m_1 - m_2}{m_1 m_2}\mathbf{p}_{\mathbf{r}} \cdot [\mathbf{r} \cdot \nabla\phi(\mathbf{R})]\mathbf{p}_{\mathbf{r}}
\end{aligned}
\tag{3.12}
$$

describes the internal dynamics of the atom, both modified in comparison to Ref. [1]. Here we have included the term $2\gamma\frac{\phi(\mathbf{R})}{c^2}\frac{\mathbf{p}_{\mathbf{r}}^2}{2\mu}$ into $H_{\text{A,new}}$ since it can be combined with $\frac{\mathbf{p}_{\mathbf{r}}^2}{2\mu}$ from H_{A} into

$$
\frac{\mathbf{p}_{\mathbf{r}}^2}{2\mu}\left[1 + 2\gamma\frac{\phi(\mathbf{R})}{c^2}\right] = \frac{{}^{(3)}g_{\mathbf{R}}^{-1}(\mathbf{p}_{\mathbf{r}}, \mathbf{p}_{\mathbf{r}})}{2\mu},
\tag{3.13}
$$

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

The terms H_{AL} and H_{L} describing, respectively, the atom-light interaction and the electromagnetic field are not changed compared to Ref. [1]; and the final summand

$$
H_{\text{X,new}} = H_{\text{X}} + \frac{2\gamma + 1}{2Mc^2}\{\mathbf{P} \cdot [\mathbf{r} \cdot \nabla\phi(\mathbf{R})]\mathbf{p}_{\mathbf{r}} + \text{H.c.}\} \tag{3.14}
$$

containing "cross terms" coupling the internal degrees of freedom to the central momentum $\mathbf{P}$ gains an additional term.

Note that if we assume that the gravitational potential ϕ vary slowly over the extension of the atom, we can neglect the terms $\mathbf{r} \cdot \nabla \phi(\mathbf{R})$.

IV. 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. In the following Sec. V we will then combine all couplings into a single Hamiltonian.

A. Solution of the gravitationally modified Maxwell equations

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

$$S_{\text{em}} = \int dt \, d^3\mathbf{x} \sqrt{-g} \left(-\frac{1}{4\mu_0} F_{\text{tot}.\mu\nu} F_{\text{tot}.}^{\mu\nu} + J^\mu A_{\text{tot}.\mu} \right), \quad (4.1)$$

where g denotes the determinant of the matrix $(g_{\mu\nu})$ of components of the metric, $J = J^\mu \partial_\mu$ is the 4-current "density" vector field, $A_{\text{tot}.} = A_{\text{tot}.\mu} dx^\mu$ is the (total[4]) electromagnetic 4-potential form and $dA_{\text{tot}.} = F_{\text{tot}.} = F_{\text{tot}.\mu\nu} dx^\mu \otimes dx^\nu = (\partial_\mu A_{\text{tot}.\nu} - \partial_\nu A_{\text{tot}.\mu}) dx^\mu \otimes dx^\nu$ 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 [20] to a general spacetime metric [21,22].

Note that J^μ are the components of a proper vector field and not of a density; their relation to the 4-current *density* with components j^μ, in terms of which the interaction part of the action takes the form $\int dt \, d^3\mathbf{x} \, j^\mu A_{\text{tot}.\mu}$, is given by

$$J^\mu = \frac{1}{\sqrt{-g}} j^\mu. \quad (4.2)$$

The current density of our system of two particles is given by[5]

$$j^\mu(t, \mathbf{x}) = \sum_{i=1}^{2} e_i \delta^{(3)}[\mathbf{x} - \mathbf{r}_i(t)] \dot{r}_i^\mu(t), \quad (4.3)$$

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

$$\rho := \frac{1}{c} j^0. \quad (4.4)$$

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

$$\nabla_\mu F_{\text{tot}.}^{\mu\nu} = -\mu_0 J^\nu \quad (4.5)$$

in terms of the current vector field, or

$$\nabla_\mu F_{\text{tot}.}^{\mu\nu} = -\mu_0 \frac{1}{\sqrt{-g}} j^\nu \quad (4.6)$$

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

$$\nabla^\mu F_{\text{tot}.\mu\nu} = -\mu_0 \frac{1}{\sqrt{-g}} j_\nu \quad (4.7)$$

instead.

From now on we employ the approximation that over the extension of the atom, the gravitational field ϕ is constant. This implies that all partial derivatives of the components of the metric vanish, such that the Christoffel symbols vanish and all covariant derivatives are given just by partial derivatives. Furthermore, we employ the Coulomb gauge $\nabla^i A_{\text{tot}.i} = 0$. Then, the Maxwell equations (4.7) become

$$-\mu_0 \frac{1}{\sqrt{-g}} j_\nu = g^{\mu\rho} \partial_\mu \partial_\rho A_{\text{tot}.\nu} - g^{0\rho} \partial_\nu \partial_\rho A_{\text{tot}.0}. \quad (4.8)$$

We now split the electromagnetic potential into "internal" and "external" parts, as done in [1], i.e., the part generated by our system of moving particles and that corresponding to external electromagnetic fields: We have $A_{\text{tot}.\mu} = \mathcal{A}_\mu + A_\mu$, where we adopt the Coulomb gauge for both the external part A_μ and the internal part $\mathcal{A}_\mu$. The external potential A_μ is assumed as given and satisfying the vacuum Maxwell equations, and the internal potential satisfies the Maxwell equations for the internal current density (4.3):

$$-\mu_0 \frac{1}{\sqrt{-g}} j_\nu = g^{\mu\rho} \partial_\mu \partial_\rho \mathcal{A}_\nu - g^{0\rho} \partial_\nu \partial_\rho \mathcal{A}_0. \quad (4.9)$$

Similarly, we write $F_{\text{tot}.\mu\nu} = \mathcal{F}_{\mu\nu} + F_{\mu\nu}$, where $\mathcal{F} = d\mathcal{A}$ is the internal and $F = dA$ is the external field tensor.

Inserting the PPN metric (2.2), the 0-component of the Maxwell equations (4.9) reads as follows:

$$\begin{aligned}
& -\mu_0 \frac{1}{\sqrt{-g}} j_0 \\
&= g^{\mu\rho} \partial_\mu \partial_\rho \mathcal{A}_0 - g^{0\rho} \partial_0 \partial_\rho \mathcal{A}_0 \\
&= g^{a\rho} \partial_a \partial_\rho \mathcal{A}_0 \\
&= c^{-1} g^{0a} \partial_t \partial_a \mathcal{A}_0 + g^{ab} \partial_a \partial_b \mathcal{A}_0 \\
&= \left(1 + 2\gamma \frac{\phi}{c^2} \right) \Delta \mathcal{A}_0 + O(c^{-4}). \quad (4.10)
\end{aligned}$$

Here $\Delta = \delta^{ab} \partial_a \partial_b$ denotes the "flat" spatial Laplace operator with respect to the spatial Euclidean metric defined by the background structures (flat Minkowski metric and preferred timelike vector field).

Now, using[6] $1/\sqrt{-g} = 1 + (3\gamma - 1)\frac{\phi}{c^2} + O(c^{-4})$, this equation is equivalent to

$$\Delta \mathcal{A}_0 = -\left[1 + (\gamma - 1)\frac{\phi}{c^2} \right] \mu_0 j_0 + O(c^{-4}). \quad (4.11)$$

---

[4]We will later decompose the field into internal and external contributions, hence the label "total."

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

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

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

---

[6]The determinant of the spatial metric is $\det(g_{ab}) =: {}^{(3)}g = 1 - 6\gamma \frac{\phi}{c^2} + O(c^{-4})$, and so minus the determinant of the metric is $-g = {}^{(3)}g/(-g^{00}) = [1 - 6\gamma \frac{\phi}{c^2} + O(c^{-4})][1 + 2\frac{\phi}{c^2} + O(c^{-4})] = 1 - 2(3\gamma - 1)\frac{\phi}{c^2} + O(c^{-4})$, implying $\sqrt{-g} = 1 - (3\gamma - 1)\frac{\phi}{c^2} + O(c^{-4})$.

Rewriting $j_0 = -(1 + 2\frac{\phi}{c^2})j^0 + O(c^{-4})$, recalling the charge density (4.4) and introducing the internal electric scalar potential

$$\phi_{\text{el.}} := -c\mathcal{A}_0, \tag{4.12}$$

we arrive at the Poisson equation for the electric potential:

$$\Delta\phi_{\text{el.}} = -\frac{1}{\varepsilon_0}\left[1 + (\gamma + 1)\frac{\phi}{c^2}\right]\rho + O(c^{-3}). \tag{4.13}$$

The a component of the Maxwell equations (4.9) is

$$-\mu_0\frac{1}{\sqrt{-g}}j_a$$
$$= g^{\mu\rho}\partial_\mu\partial_\rho\mathcal{A}_a - g^{0\rho}\partial_a\partial_\rho\mathcal{A}_0$$
$$= g^{\mu\rho}\partial_\mu\partial_\rho\mathcal{A}_a - \left[1 - 2\frac{\phi}{c^2} + O(c^{-4})\right]\varepsilon_0\mu_0\partial_a\partial_t\phi_{\text{el.}} \tag{4.14}$$

With $g^{\mu\rho}\partial_\mu\partial_\rho\mathcal{A}_a = (1 + 2\gamma\frac{\phi}{c^2})\Delta\mathcal{A}_a - c^{-2}\partial_t^2\mathcal{A}_a + O(c^{-4}) = (1 + 2\gamma\frac{\phi}{c^2})(\Delta - c^{-2}\partial_t^2)\mathcal{A}_a + O(c^{-4})$, this is equivalent to

$$(\Delta - c^{-2}\partial_t^2)\mathcal{A}_a$$
$$= -\mu_0\left\{\left[1 + (\gamma - 1)\frac{\phi}{c^2}\right]j_a\right.$$
$$\left. - \left[1 - 2(\gamma + 1)\frac{\phi}{c^2}\right]\varepsilon_0\partial_a\partial_t\phi_{\text{el.}}\right\} + O(c^{-4}). \tag{4.15}$$

Rewriting $j_a = (1 - 2\gamma\frac{\phi}{c^2})j^a + O(c^{-4})$ and introducing the internal vector potential[7] $\mathcal{A} = \mathcal{A}^\perp$ in $\mathcal{A}_\mu = (-\phi_{\text{el.}}/c, \mathcal{A}^\perp)$, the wave equation for this potential reads as follows:

$$(\Delta - c^{-2}\partial_t^2)\mathcal{A}^\perp$$
$$= -\mu_0\left\{\left[1 - (\gamma + 1)\frac{\phi}{c^2}\right]\mathbf{j}\right.$$
$$\left. - \left[1 - 2(\gamma + 1)\frac{\phi}{c^2}\right]\varepsilon_0\nabla\partial_t\phi_{\text{el.}}\right\} + O(c^{-4}). \tag{4.16}$$

Now solving Eqs. (4.13) and (4.16) for the internal potentials as in Appendix A of Ref. [1], we see that to leading post-Newtonian order we arrive at the same potentials as in the nongravitational case, up to prefactors: We have

$$\phi_{\text{el.}} = \left[1 + (\gamma + 1)\frac{\phi}{c^2}\right]\phi_{\text{el.,ng}} \tag{4.17}$$

and

$$\mathcal{A}^\perp = \left[1 - (\gamma + 1)\frac{\phi}{c^2}\right]\mathcal{A}_{\text{ng}}^\perp, \tag{4.18}$$

where the suffix "ng" stands for "nongravitational," i.e., for the solutions from (A[1].A1) and (A[1].A3). Since we are assuming the absence of external charges, the external electric scalar potential A_0 vanishes due to the "external" equivalent

_____

[7]It is a transverse vector field because of the Coulomb gauge condition.

of (4.10); and we introduce the external transverse vector potential $\mathbf{A} = \mathbf{A}^\perp$ as $A_\mu = (0, \mathbf{A}^\perp)$.

B. Computation of the electromagnetic Lagrangian

We will now use the obtained potentials to compute the electromagnetic Lagrangian

$$L_{\text{em}} = \int d^3\mathbf{x}\left(-\frac{1}{4\mu_0}\sqrt{-g}F_{\text{tot.}\mu\nu}F_{\text{tot.}}^{\mu\nu} + j^\mu A_{\text{tot.}\mu}\right), \tag{4.19}$$

which follows from the action (4.1). For the internal kinetic Maxwell term, we obtain

$$-\frac{1}{4\mu_0}\int d^3\mathbf{x}\sqrt{-g}\mathcal{F}_{\mu\nu}\mathcal{F}^{\mu\nu}$$
$$= -\frac{1}{2\mu_0}\int d^3\mathbf{x}\sqrt{-g}\partial_\mu\mathcal{A}_\nu\mathcal{F}^{\mu\nu}$$
$$\text{(P.I.)}$$
$$= \frac{1}{2\mu_0}\int d^3\mathbf{x}\sqrt{-g}\mathcal{A}_\nu\nabla_\mu\mathcal{F}^{\mu\nu}$$
$$- \frac{1}{2\mu_0}\int d^3\mathbf{x}[\sqrt{-g}\partial_0\mathcal{A}_\nu\mathcal{F}^{0\nu} + \mathcal{A}_\nu\partial_0(\sqrt{-g}\mathcal{F}^{0\nu})]$$
$$= -\frac{1}{2}\int d^3\mathbf{x}\mathcal{A}_\nu j^\nu$$
$$- \frac{1}{2\mu_0}\int d^3\mathbf{x}[\sqrt{-g}\partial_0\mathcal{A}_a(\nabla^0\mathcal{A}^a - \nabla^a\mathcal{A}^0)$$
$$+ \mathcal{A}_a\partial_0(\sqrt{-g}\nabla^0\mathcal{A}^a - \sqrt{-g}\nabla^a\mathcal{A}^0)]$$
$$\text{(P.I., } \partial_i g_{\mu\nu} = 0, \nabla^i\mathcal{A}_i = 0)$$
$$= -\frac{1}{2}\int d^3\mathbf{x}\mathcal{A}_\nu j^\nu - \frac{1}{2\mu_0}\int d^3\mathbf{x}\sqrt{-g}(\partial_0\mathcal{A}_a\partial^0\mathcal{A}^a$$
$$+ \mathcal{A}_a\partial_0\partial^0\mathcal{A}^a) + O(c^{-4}), \tag{4.20}$$

where in the last step, to perform the partial integration, we used that the metric is diagonal up to $O(c^{-4})$. Inserting the PPN metric, we obtain

$$-\frac{1}{2\mu_0}\int d^3\mathbf{x}\sqrt{-g}(\partial_0\mathcal{A}_a\partial^0\mathcal{A}^a + \mathcal{A}_a\partial_0\partial^0\mathcal{A}^a)$$
$$= -\frac{\varepsilon_0}{2}\int d^3\mathbf{x}\sqrt{-g}g^{00}g^{ab}(\partial_t\mathcal{A}_a\partial_t\mathcal{A}_b + \mathcal{A}_a\partial_t^2\mathcal{A}_b) + O(c^{-4})$$
$$= \left[1 - (\gamma + 1)\frac{\phi}{c^2}\right]\frac{\varepsilon_0}{4}\int d^3\mathbf{x}\partial_t^2\mathcal{A}^2 + O(c^{-4}). \tag{4.21}$$

Thus, combining (4.20) and (4.21), the "purely internal" contribution of electromagnetism to the Lagrangian, including the explicit coupling term of the internal potential to the current, is

$$L_{\text{em,int.}} = \int d^3\mathbf{x}\left(-\frac{1}{4\mu_0}\sqrt{-g}\mathcal{F}_{\mu\nu}\mathcal{F}^{\mu\nu} + j^\mu\mathcal{A}_\mu\right)$$
$$= \frac{1}{2}\int d^3\mathbf{x}j^\mu\mathcal{A}_\mu$$
$$+ \left[1 - (\gamma + 1)\frac{\phi}{c^2}\right]\frac{\varepsilon_0}{4}\int d^3\mathbf{x}\partial_t^2\mathcal{A}^2 + O(c^{-4}). \tag{4.22}$$

Following Appendix B in Ref. [1], we will neglect the second integral in this expression.[8]

For computing the other (purely external and mixed external-internal) contributions to the total electromagnetic Lagrangian (4.19), it is easiest to first rewrite the total kinetic Maxwell term. Using the PPN metric, but not the gauge condition, and writing $A_{\text{tot}.\mu} = (-\phi_{\text{el.,tot.}}/c, \mathbf{A}_{\text{tot.}})$, we have

$$
-\frac{1}{4\mu_0}\sqrt{-g}F_{\text{tot}.\mu\nu}F_{\text{tot.}}^{\mu\nu}
$$
$$
= \frac{\varepsilon_0}{2}\sqrt{-g}[-g^{00}g^{ab}(\partial_t A_{\text{tot}.a} + \partial_a \phi_{\text{el.,tot.}})(\partial_t A_{\text{tot}.b} + \partial_b \phi_{\text{el.,tot.}})
$$
$$
- c^2(g^{ab}g^{cd} - g^{ad}g^{cb})\partial_a A_{\text{tot}.c}\partial_b A_{\text{tot}.d})] + O(c^{-4})
$$
$$
= \frac{\varepsilon_0}{2}\left\{\left[1 - (\gamma + 1)\frac{\phi}{c^2}\right](\partial_t\mathbf{A}_{\text{tot.}} + \boldsymbol{\nabla}\phi_{\text{el.,tot.}})^2\right.
$$
$$
\left. - c^2\left[1 + (\gamma + 1)\frac{\phi}{c^2}\right](\boldsymbol{\nabla}\times\mathbf{A}_{\text{tot.}})^2\right\} + O(c^{-4}). \tag{4.23}
$$

We recall that, as explained in Sec. II C, the boldface nabla symbol $\boldsymbol{\nabla}$ denotes the three-tuple of *partial* derivatives, and $\boldsymbol{\nabla}\times\mathbf{A}_{\text{tot.}}$ denotes the "component-wise curl" of $\mathbf{A}_{\text{tot.}}$. Both of these operations are well defined (independent of coordinates) once we have introduced the background structures (flat Minkowski metric and preferred timelike vector field).

The internal-internal term of (4.23) was considered above in (4.22). The external-external term gives ($\phi_{\text{el.,tot.}}$ is internal, and $\mathbf{A} = \mathbf{A}^\perp$ is transverse because of the gauge condition)

$$
L_{\text{em,ext.}} = -\frac{1}{4\mu_0}\int d^3\mathbf{x}\sqrt{-g}F_{\mu\nu}F^{\mu\nu}
$$
$$
= \frac{\varepsilon_0}{2}\int d^3\mathbf{x}\left\{\left[1 - (\gamma + 1)\frac{\phi}{c^2}\right](\partial_t\mathbf{A}^\perp)^2\right.
$$
$$
\left. - c^2\left[1 + (\gamma + 1)\frac{\phi}{c^2}\right](\boldsymbol{\nabla}\times\mathbf{A}^\perp)^2\right\} + O(c^{-4}), \tag{4.24}
$$

and the external-internal mixed term plus the interaction of the external potential with the current is (using partial integration and the gauge condition to get rid of the $\partial_t\mathbf{A}^\perp\cdot\boldsymbol{\nabla}\phi_{\text{el.}}$ term)

$$
L_{\text{em,ext.-int.}}
$$
$$
= \int d^3\mathbf{x}\, j^\mu A_\mu - \frac{1}{2\mu_0}\int d^3\mathbf{x}\sqrt{-g}\mathcal{F}_{\mu\nu}F^{\mu\nu}
$$
$$
= \int d^3\mathbf{x}\, j^\mu A_\mu
$$
$$
+ \varepsilon_0\int d^3\mathbf{x}\left\{\left[1 - (\gamma + 1)\frac{\phi}{c^2}\right](\partial_t\boldsymbol{\mathcal{A}}^\perp)\cdot(\partial_t\mathbf{A}^\perp)\right.
$$
$$
\left. - c^2\left[1 + (\gamma + 1)\frac{\phi}{c^2}\right](\boldsymbol{\nabla}\times\boldsymbol{\mathcal{A}}^\perp)\cdot(\boldsymbol{\nabla}\times\mathbf{A}^\perp)\right\} + O(c^{-4}). \tag{4.25}
$$

---

[8]Quoting Appendix B in Ref. [1], it leads to terms "proportional to the electrostatic energy of the atom divided by $m_i c^2$ times $|\mathbf{r}_j|^2/c^2$, which goes beyond our level of approximation."

Following Appendix B in Ref. [1], we will neglect the second integral also in this expression, since it is related to formally diverging backreaction terms.

Adding the Lagrangians (4.22), (4.24), and (4.25), the total post-Newtonian electromagnetic Lagrangian (with the above-mentioned neglected points following Ref. [1]) reads

$$
L_{\text{em}} = \frac{1}{2}\int d^3\mathbf{x}\,(\mathbf{j}\cdot\boldsymbol{\mathcal{A}}^\perp - \rho\phi_{\text{el.}}) + \int d^3\mathbf{x}\,\mathbf{j}\cdot\mathbf{A}^\perp
$$
$$
+ \frac{\varepsilon_0}{2}\int d^3\mathbf{x}\left\{\left[1 - (\gamma + 1)\frac{\phi}{c^2}\right](\partial_t\mathbf{A}^\perp)^2\right.
$$
$$
\left. - c^2\left[1 + (\gamma + 1)\frac{\phi}{c^2}\right](\boldsymbol{\nabla}\times\mathbf{A}^\perp)^2\right\} + O(c^{-4}). \tag{4.26}
$$

Inserting the internal potentials (4.17) and (4.18) as well as the current and charge densities (4.3) and (4.4) and dropping infinite self-interaction terms for the internal part of the electromagnetic Lagrangian we obtain

$$
\frac{1}{2}\int d^3\mathbf{x}\,(\mathbf{j}\cdot\boldsymbol{\mathcal{A}}^\perp - \rho\phi_{\text{el.}})
$$
$$
= -\left[1 + (\gamma + 1)\frac{\phi}{c^2}\right]\frac{e_1 e_2}{4\pi\varepsilon_0 r} + \left[1 - (\gamma + 1)\frac{\phi}{c^2}\right]\frac{e_1 e_2}{8\pi\varepsilon_0 c^2}
$$
$$
\times\left[\frac{\dot{\mathbf{r}}_1\cdot\dot{\mathbf{r}}_2}{r} + \frac{(\dot{\mathbf{r}}_1\cdot\mathbf{r})(\dot{\mathbf{r}}_2\cdot\mathbf{r})}{r^3}\right] + O(c^{-4})
$$
$$
= -\left[1 + (\gamma + 1)\frac{\phi}{c^2}\right]\frac{e_1 e_2}{4\pi\varepsilon_0 r}
$$
$$
+ \frac{e_1 e_2}{8\pi\varepsilon_0 c^2}\left[\frac{\dot{\mathbf{r}}_1\cdot\dot{\mathbf{r}}_2}{r} + \frac{(\dot{\mathbf{r}}_1\cdot\mathbf{r})(\dot{\mathbf{r}}_2\cdot\mathbf{r})}{r^3}\right] + O(c^{-4}). \tag{4.27}
$$

V. THE TOTAL HAMILTONIAN INCLUDING ALL INTERACTIONS

In this section we collect all previous findings and combine them into the total Hamiltonian that characterizes the dynamics of our two-particle system that is now also exposed to a nontrivial 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 reexpressed in terms of the physical spacetime metric g.

A. 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 Sec. III while including the "gravitational corrections" to electromagnetism obtained in Sec. IV.

Comparing the gravitationally corrected electromagnetic Lagrangian (4.26) and (4.27) to the one without gravitational field ($\phi = 0$), we see that at our order of approximation the only differences occur in the external electromagnetic term and the internal Coulomb interaction term. Thus, when calculating the Hamiltonian, we have to only take care of these changes compared to the discussion of Sec. III.

The canonical momentum conjugate to $\mathbf{A}^\perp$ is

$$\boldsymbol{\Pi}^\perp = \frac{\delta L_{\text{em}}}{\delta(\partial_t \mathbf{A}^\perp)} = \varepsilon_0 \left[1 - (\gamma + 1)\frac{\phi}{c^2} \right] \partial_t \mathbf{A}^\perp + O(c^{-4}),$$
(5.1)

and the Hamiltonian for the external electromagnetic field thus is

$$H_{\text{em,ext.}} = \int d^3\mathbf{x} \, \boldsymbol{\Pi}^\perp \cdot \partial_t \mathbf{A}^\perp - L_{\text{em,ext}}$$

$$= \frac{\varepsilon_0}{2} \int d^3\mathbf{x} \left[1 + (\gamma + 1)\frac{\phi}{c^2} \right] [(\boldsymbol{\Pi}^\perp/\varepsilon_0)^2$$

$$+ c^2 (\nabla \times \mathbf{A}^\perp)^2] + O(c^{-4}).$$
(5.2)

Thus, when including the new corrections, the classical Hamiltonian will be the same as given by (3.3) and (A[1].12*), except for the Coulomb term and the external electromagnetic field energy both gaining the prefactor $[1 + (\gamma + 1)\frac{\phi}{c^2}]$. The same will be true after quantizing and performing the PZW transformation and electric dipole approximation: Using the same expression (A[1].14*) for the PZW operator, we arrive at the multipolar Hamiltonian from (3.4) and (A[1].23*), except for this prefactor in the corresponding terms.

Now transforming to central and relative coordinates, as in going from (3.4) and (A[1].23*) to (3.9) and (A[1].25*), the same stays true; we just have to keep in mind that the relation between the electromagnetic canonical momentum $\boldsymbol{\Pi}^\perp$ and the transverse external "coordinate electric field" $\mathbf{E}^\perp_{\text{coord.}} = -\partial_t \mathbf{A}^\perp$ now also gains an additional factor. Including this, the electric field-dipole interaction term again has the form $-\mathbf{d} \cdot \mathbf{E}^\perp_{\text{coord.}}(\mathbf{R})$ as in the nongravitational case, but the dipole polarization self-interaction term $\frac{1}{2\varepsilon_0} \int d^3\mathbf{x} \, \mathcal{P}_d^{\perp 2}$ in H_{AL} gains a prefactor (since it arises from the PZW-transformed external field energy).

Thus, comparing to the discussion of Sec. III, the external electromagnetic field energy, the $\mathcal{P}_d^{\perp 2}$ term in H_{AL}, and the Coulomb term are multiplied by the factor $[1 + (\gamma + 1)\frac{\phi}{c^2}]$, and we arrive at the following total Hamiltonian:

$$H_{\text{[com],final}} = H_{\text{C,final}} + H_{\text{A,final}} + H_{\text{AL,final}} + H_{\text{L,final}} + H_X,$$
(5.3a)

$$H_{\text{C,final}} = H_{\text{C,new}} - \frac{1}{c^2} \frac{e^2}{4\pi\varepsilon_0 r} \phi(\mathbf{R}),$$
(5.3b)

$$H_{\text{A,final}} = H_{\text{A,new}} - \gamma \frac{1}{c^2} \frac{e^2}{4\pi\varepsilon_0 r} \phi(\mathbf{R}),$$
(5.3c)

$$H_{\text{AL,final}} = H_{\text{AL}} + \frac{1}{2\varepsilon_0} \int d^3\mathbf{x} \, (\gamma + 1)\frac{\phi}{c^2} \mathcal{P}_d^{\perp 2},$$
(5.3d)

$$H_{\text{L,final}} = \frac{\varepsilon_0}{2} \int d^3\mathbf{x} \left[1 + (\gamma + 1)\frac{\phi}{c^2} \right]$$

$$\times [(\boldsymbol{\Pi}^\perp/\varepsilon_0)^2 + c^2(\nabla \times \mathbf{A}^\perp)^2].$$
(5.3e)

Here we have included the term $-\gamma \frac{1}{c^2} \frac{e^2}{4\pi\varepsilon_0 r} \phi(\mathbf{R})$ into $H_{\text{A,final}}$ since it can be combined with the original Coulomb term from H_A into

$$-\frac{e^2}{4\pi\varepsilon_0 r} \left[1 + \gamma \frac{\phi(\mathbf{R})}{c^2} \right] = -\frac{e^2}{4\pi\varepsilon_0 \sqrt{{}^{(3)}g_{\mathbf{R}}(\mathbf{r},\mathbf{r})}},$$
(5.4)

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

Note that we neglected the terms $\mathbf{r} \cdot \nabla\phi(\mathbf{R})$ (since we assumed ϕ to be constant over the extension of the atom), thus arriving at the same cross terms H_X as in (A[1].25f); similarly, the corresponding term from $H_{\text{A,new}}$ (3.12) can be neglected.

To correctly interpret the atom-light interaction Hamiltonian (5.3d), one has to keep in mind that the field variables $\mathbf{E}^\perp$ and $\mathbf{B}$ in H_{AL} (A[1].25d*) are the *coordinate* components $-\partial_t \mathbf{A}^\perp$ and $\nabla \times \mathbf{A}^\perp$, respectively, which do not refer to an orthonormal frame in the physical spacetime metric g in the presence of gravitational fields. This issue will be discussed in more detail in Sec. V C.

Since the cross terms H_X are the same as in Ref. [1], we could now introduce new coordinates $\mathbf{Q}, \mathbf{q}, \mathbf{p}$ literally as in (A[1].26) to eliminate these cross terms. Since the gravitational correction terms are of order $O(c^{-2})$, for them this change into the new coordinates would just amount to the replacements $\mathbf{R} \to \mathbf{Q}, \mathbf{r} \to \mathbf{q}, \mathbf{p}_r \to \mathbf{p}$ 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.

B. The system as a composite point particle

Fully writing out the central and internal Hamiltonian (5.3b), (5.3c), we obtain

$$H_{\text{C,final}} = \frac{\mathbf{P}^2}{2M} \left[1 - \frac{1}{Mc^2}\left(\frac{\mathbf{p}_r^2}{2\mu} + \frac{e_1 e_2}{4\pi\varepsilon_0 r} \right) \right]$$

$$+ \left[M + \frac{1}{c^2}\left(\frac{\mathbf{p}_r^2}{2\mu} + \frac{e_1 e_2}{4\pi\varepsilon_0 r} \right) \right] \phi(\mathbf{R})$$

$$- \frac{\mathbf{P}^4}{8M^3 c^2} + \frac{2\gamma + 1}{2Mc^2} \mathbf{P} \cdot \phi(\mathbf{R})\mathbf{P}$$

$$+ (2\beta - 1)\frac{M\phi(\mathbf{R})^2}{2c^2},$$
(5.5)

$$H_{\text{A,final}} = \frac{{}^{(3)}g_{\mathbf{R}}^{-1}(\mathbf{p}_r, \mathbf{p}_r)}{2\mu} + \frac{e_1 e_2}{4\pi\varepsilon_0 \sqrt{{}^{(3)}g_{\mathbf{R}}(\mathbf{r},\mathbf{r})}}$$

$$- \frac{m_1^3 + m_2^3}{M^3} \frac{\mathbf{p}_r^4}{8\mu^3 c^2} + \frac{e_1 e_2}{4\pi\varepsilon_0} \frac{1}{2\mu M c^2}$$

$$\times \left(\mathbf{p}_r \cdot \frac{1}{r}\mathbf{p}_r + \mathbf{p}_r \cdot \mathbf{r}\frac{1}{r^3}\mathbf{r} \cdot \mathbf{p}_r \right),$$
(5.6)

where we combined the gravitational correction terms in $H_{\text{A,final}}$ into metrically defined kinetic energy and Coulomb terms as in (3.13), (5.4).

Comparing to the Hamiltonian of a single point particle of mass m in the PPN metric,

$$H_{\text{point}}(\mathbf{P}, \mathbf{R}; m)$$
$$= \frac{\mathbf{P}^2}{2m} + m\phi(\mathbf{R}) - \frac{\mathbf{P}^4}{8m^3c^2} + \frac{2\gamma + 1}{2mc^2}\mathbf{P} \cdot \phi(\mathbf{R})\mathbf{P}$$
$$+ (2\beta - 1)\frac{m\phi(\mathbf{R})^2}{2c^2}, \qquad (5.7)$$

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

$$H_{\text{C,final}} = H_{\text{point}}\left(\mathbf{P}, \mathbf{R}; M + \frac{H_{\text{A,final}}}{c^2}\right), \qquad (5.8)$$

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 comprises 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 (3.13) and the Coulomb interaction (5.4) in terms of the physical metric g, the above conclusion could not have resulted. Rather, we would have had to replace the inertial mass of the "composite particle" by $M + \frac{H_A}{c^2}$ and the gravitational mass by $M + (2\gamma + 1)\frac{\mathbf{p}^2}{2\mu c^2} + (\gamma + 1)\frac{e_1 e_2}{4\pi\varepsilon_0 qc^2} = M + \frac{H_A}{c^2} + \gamma(2\frac{\mathbf{p}^2}{2\mu c^2} + \frac{e_1 e_2}{4\pi\varepsilon_0 qc^2})$, 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 Ref. [8].

The quantities $\vec{p}'^2$ and r' entering the Hamiltonian [Eq. (18)] in Ref. [8], which are, in the language of Ref. [8], the square of the internal momentum and the distance "in the CM rest frame," are nothing but the geometric expressions $^{(3)}g_{\mathbf{R}}^{-1}(\mathbf{p_r}, \mathbf{p_r})$ and $\sqrt{^{(3)}g_{\mathbf{R}}(\mathbf{r}, \mathbf{r})}$ from above, measured using the physical metric of space. The internal Hamiltonian (5.6) thus consists of kinetic and Coulomb interaction energies in terms of the physical geometry, in agreement with the expressions from Ref. [8], as well as the expected special-relativistic and "Darwin" corrections.[9]

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[9]Since these corrections are themselves of order $1/c^2$, the deviations of the physical from the flat metric do not enter here.

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

The expressions derived above in (5.3) include components of the 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 chosen background structure (η, u). This means that $u = \partial/\partial t$ and $\eta = \eta_{\mu\nu}\,dx^\mu \otimes dx^\nu$ with $(\eta_{\mu\nu}) = \text{diag}(-1, 1, 1, 1)$. The corresponding local reference frames $\{\partial_\mu := \partial/\partial x^\mu \mid \mu = 0, 1, 2, 3\}$ are orthonormal with respect to η but not with respect to the physical metric g.

In this subsection we will reexpress our findings in terms of components with respect to orthonormal frames with respect to g, 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 nonorthonormal 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 physical significance, from the expressions involving the components alone, without at the same time having to recall the values of the metric components as well.

The full atom-light interaction Hamiltonian $H_{\text{AL,final}}$ (5.3d) reads

$$H_{\text{AL,final}} = -\mathbf{d} \cdot \mathbf{E}_{\text{coord.}}^{\perp}(\mathbf{R}) + \frac{1}{2M}\{\mathbf{P} \cdot [\mathbf{d} \times \mathbf{B}_{\text{coord.}}(\mathbf{R})] + \text{H.c.}\}$$
$$- \frac{m_1 - m_2}{4m_1 m_2}\{\mathbf{p_r} \cdot [\mathbf{d} \times \mathbf{B}_{\text{coord.}}(\mathbf{R})] + \text{H.c.}\}$$
$$+ \frac{1}{8\mu}[\mathbf{d} \times \mathbf{B}_{\text{coord.}}(\mathbf{R})]^2$$
$$+ \frac{1}{2\varepsilon_0}\int d^3\mathbf{x}\left[1 + (\gamma + 1)\frac{\phi}{c^2}\right]\mathcal{P}_d^{\perp 2}(\mathbf{x}, t), \quad (5.9)$$

where $\mathbf{E}_{\text{coord.}}^{\perp} = -\partial_t \mathbf{A}^{\perp}$ and $\mathbf{B}_{\text{coord.}}^{\perp} = \nabla \times \mathbf{A}^{\perp}$, i.e., $E_{\text{coord.}a} = cF_{a0}$ and $B_{\text{coord.}}^a = \varepsilon^{abc}F_{bc}$, are given by the coordinate components of the electromagnetic field tensor that refer to nonorthonormal frames ∂_μ. Since our metrics η and g are both diagonal in the coordinates used and to the order of approximation employed here, we simply need to divide ∂_μ by the square root of the modulus of $g_{\mu\mu}$ (no summation) in order to get an orthonormal frame $e_{\underline{\mu}}$ for g, called a "tetrad":

$$e_{\underline{0}} = \frac{1}{\sqrt{-g_{00}}}\partial_0 = \left(1 - \frac{\phi}{c^2}\right)\partial_0, \qquad (5.10\text{a})$$

$$e_{\underline{a}} = \frac{1}{\sqrt{g_{aa}}}\partial_a = \left(1 + \gamma\frac{\phi}{c^2}\right)\partial_a. \qquad (5.10\text{b})$$

Note that from now on underlined indices refer to the tetrad ("physical components"), nonunderlined ones to the coordinate basis ("coordinate components").

The "physical components" of the electric and magnetic fields with respect to the tetrad are given in terms of the tetrad components of the field tensor through

$$E_{\text{phys.}\underline{a}} = cF_{\underline{a}0}, \qquad B_{\text{phys.}}^{\underline{a}} = \sum_{b,c=1}^{3}\varepsilon^{abc}F_{\underline{b}\underline{c}}, \qquad (5.11)$$

where ε^{abc} is the totally antisymmetric symbol. This can be understood in a more geometric way: Denoting by $\tilde{\varepsilon}^{\underline{abc}}$ the tetrad components of the spatial volume form $\tilde{\varepsilon}$ that is induced by the physical metric g (instead of the spatial volume form ε induced by the background metric η), we have the numerical identity

$$\tilde{\varepsilon}^{\underline{abc}} = \varepsilon^{abc} \tag{5.12}$$

since the tetrad basis vectors $\{e_{\underline{a}}\}$ are orthonormal with respect to g. Thus, the magnetic field components can be written as

$$B_{\text{phys.}}^{\underline{a}} = \tilde{\varepsilon}^{\underline{abc}} F_{\underline{bc}}, \tag{5.13}$$

with clear geometric meaning. Inserting the tetrad (5.10), the components (5.11) are related to the coordinate expressions $E_{\text{coord.}a} = cF_{a0}$ and $B_{\text{coord.}}^a = \varepsilon^{abc} F_{bc}$ by

$$\mathbf{E}_{\text{phys.}} = \frac{1}{\sqrt{-g_{00}}}\left(1 + \gamma \frac{\phi}{c^2}\right)\mathbf{E}_{\text{coord.}}, \tag{5.14a}$$

$$\mathbf{B}_{\text{phys.}} = \left(1 + 2\gamma \frac{\phi}{c^2}\right)\mathbf{B}_{\text{coord.}}. \tag{5.14b}$$

Similarly, the dipole moment $d^a = \sum_{k=1,2} e_k(r_k^a - R^a)$ is defined via coordinate distances, and thus the physically significant, metric dipole moment is given by

$$d_{\text{phys.}}^{\underline{a}} = e_b^{\underline{a}} d^b = \left(1 - \gamma \frac{\phi}{c^2}\right)d^a. \tag{5.15}$$

Thus the electric dipole interaction term in the Hamiltonian takes the form

$$-\mathbf{d} \cdot \mathbf{E}_{\text{coord.}}^{\perp}(\mathbf{R}) = -\sqrt{-g_{00}(\mathbf{R})}\, \mathbf{d}_{\text{phys.}} \cdot \mathbf{E}_{\text{phys.}}^{\perp}(\mathbf{R}) \tag{5.16}$$

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 $\mathbf{R}$ instead of coordinate time [9,18].

Similarly, all the other interaction terms from (5.9) 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 $\mathbf{P}$: If the components P_a were just the components of a classical covector field (i.e., a one-form), there would be no problem in computing its tetrad components as

$$P_{\text{phys.}\underline{a}} = e_{\underline{a}}^b P_b = \left(1 - \gamma \frac{\phi}{c^2}\right)P_a. \tag{5.17}$$

However, the P_a are operators that don't commute with the center of mass position $\mathbf{R}$, such that in the application of (5.17) 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

$$\frac{1}{2M}\{\mathbf{P} \cdot [\mathbf{d} \times \mathbf{B}_{\text{coord.}}(\mathbf{R})] + \text{H.c.}\}$$

$$= \frac{1}{2M}\left\{\mathbf{P} \cdot \left[1 - \gamma \frac{\phi(\mathbf{R})}{c^2}\right][\mathbf{d}_{\text{phys.}} \times \mathbf{B}_{\text{phys.}}(\mathbf{R})] + \text{H.c.}\right\} \tag{5.18}$$

for the Röntgen term. 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 $\mathbf{P}$ of the momentum refer to the coordinate basis and the components $\mathbf{d}_{\text{phys.}}, \mathbf{B}_{\text{phys.}}$ of the dipole moment and the magnetic field refer to the tetrad.

Note that for the internal momentum $\mathbf{p_r}$, occurring in the third interaction term in (5.9), such operator ordering ambiguities do not arise, since we assumed the gravitational potential ϕ to be constant over the extension of the atom.

To the best of our knowledge, the atom-light interaction terms in the presence of gravity obtained in (5.9) and discussed above are new, save for the electric dipole coupling which was already discussed in Refs. [9,18].

Finally, expressing the external field energy (5.3e) in terms of tetrad components, we obtain

$$H_{\text{L,final}} = \frac{\varepsilon_0}{2}\int d^3\mathbf{x}\left[1 + (1 - 3\gamma)\frac{\phi}{c^2}\right]\left[\mathbf{E}_{\text{phys.}}^{\perp}{}^2 + c^2\mathbf{B}_{\text{phys.}}^2\right]$$

$$= \frac{\varepsilon_0}{2}\int d^3\mathbf{x}\sqrt{-g}\left[\mathbf{E}_{\text{phys.}}^{\perp}{}^2 + c^2\mathbf{B}_{\text{phys.}}^2\right], \tag{5.19}$$

which is the standard result of the flat-spacetime electromagnetic field energy [20] minimally coupled to gravity [21], as was to be expected.[10]

VI. A COMMENT ON THE EQUIVALENCE PRINCIPLE IN QUANTUM MECHANICS

As advertised at the end of the introduction, we now wish to come back to the less technical but conceptually all-important issue surrounding the meaning of the phrase "Equivalence Principle," in particular concerning the principle's susceptibility to be more accurately tested by genuine quantum matter. Clearly, that possibility presupposes the formulation of the Equivalence Principle in a way that is fully compatible with Quantum Mechanics. Our discussion here is motivated by our impression that this need, simple and obvious as it might seem to be, is often unduly neglected. As emphasized before, our central point of concern results from our conviction that any generally valid implementation of the Equivalence Principle into Quantum Mechanics should not be based on *a priori* assumptions concerning the state of the matter. In particular, it should not rely on semiclassical

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[10]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 Sec. II C, the approach based on the background structures enabled us to provide a direct comparison with the original calculation of Ref. [1].

notions like "wordline," which often enter discussions in a fundamental way;[11] see, e.g., Refs. [3–8]. It should also not rely on other classical formulations, like "equality of inertial and gravitational mass," for reasons discussed below.

Rather, the meaning of the Equivalence Principle is to ensure that *a single* spacetime geometry accounts for *all* matter couplings, thereby comprising all gravity phenomena on all kinds of matter; compare Ref. [10]. This does clearly not imply that all "things" (bodies, wave packets, etc.) "fall" with the same acceleration. First, in order to give a measure for the acceleration of "fall," we need to kinematically define that term; that is, we need to specify a structure on which we can read off such quantities as acceleration. In other words: we need to define a worldline. As discussed before, quantum-mechanical systems only do that in very special states. Second, even in case a worldline is approximately definable, there is no reason why it must coincide with that of another system if both start out in the same center of mass initial state. This is not even true in classical physics. The universality of free fall reduces to the equality of worldlines only in case of "test particles," idealized objects of partially opposing properties.[12] For realistic bodies, which are spinning and/or possess higher mass multipoles, the centers of mass will not define universal point-particle trajectories (i.e., geodesics). To find the equations of motion for structured bodies in arbitrary gravitational fields is, in fact, one of the most difficult challenges in General Relativity research [24]. However, as long as all deviations from the geodesic motion find their explanations in couplings to the spacetime geometry, no violation of the Equivalence Principle should be concluded. Likewise, extended wave packets in Quantum Mechanics will move in a way that depends on the higher moments of their probability distribution [25], but this does not contradict any Equivalence Principle requirement, contrary to the impression given in Ref. [25]. In that context we wish to remind the reader of our discussion in the introduction.

Finally, we also wish to comment on attempts to translate the equality of inertial and gravitational (more precisely: passive gravitational) mass into Quantum Mechanics; see, e.g., Ref. [26]. These attempts also bear the danger to prematurely conclude apparent violations, even though all the couplings are through the geometry only. In fact, it seems to us that those attempts suffer from a logical flaw that we now wish to briefly characterize.

First the positive results: It is an elementary theorem in ordinary Quantum Mechanics that, given a spatially homoge-

neous but arbitrarily time dependent force field, any solution to the Schrödinger equation in that field corresponds to a solution of the force-free Schrödinger equation written in the coordinates of a frame that freely falls according to the classical equations of motion in the given force field. This is, e.g., proven in Ref. [27]. If the force field is that of Newtonian gravity, such that the classical trajectory only depends on the ratio of the inertial to the gravitational mass, then the motion of any wave packet is that of a free Schrödinger wave in a *universally* (i.e., the same for all wave functions and all particles with the same ratio of inertial and gravitational mass) falling frame. In that sense there is no observational difference between a falling wave packet in a homogeneous gravitational field and a free wave packet without gravity viewed from a frame that rigidly moves with equal but opposite acceleration to that determined by the gravity field. This precisely corresponds to the Equivalence Principle for homogeneous fields in Newtonian gravity which we therefore see to extend to Quantum Mechanics.

In Classical Mechanics, we can extend the universality of free fall to nonhomogeneous fields if we restrict attention to pointlike test particles. Their equation of motion then guarantees the universality of free fall, given that their inertial equals their gravitational mass. This shows that we need the particular equations of motion to provide the logical link between the universality of free fall on one side and the equality of the inertial and gravitational mass on the other. As such the latter equality does not tell us anything if this link is not provided. That, in our opinion, is the flaw in any premature identification of the weak Equivalence Principle with the equality of inertial and gravitational mass (leaving alone the ambiguity to define the latter in non-Newtonian situations). In particular this applies to Quantum Mechanics, where neither the notion of a "test particle" exists, nor does there exist an obvious worldline the equation of which could provide the sought-for link. So, for general states, it remains logically unclear what a possible equality of somehow defined inertial and gravitational masses implies for the universality of free fall, though it might make contextual sense for special states. However, that state dependency means that it cannot be used as a fundamental principle.

VII. CONCLUSIONS

In this paper we extended the calculation of Ref. [1] of a Hamiltonian describing an electromagnetically interacting two-particle system to nonflat spacetimes representing weak gravitational fields in the sense of being close to Minkowski spacetime. 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 Ref. [1], but the latter are new to the best of our knowledge. Our first principles were the special-relativistic action of two equally but oppositely charged particles with their electromagnetic interaction up to, and including, terms of order c^{-2}, the minimal coupling scheme for gravity, and canonical quantization applied to the degrees of freedom in the Hamiltonian formalism. As in Ref. [1] we neglected all terms of third and higher order in c^{-1}, which physically means that we neglected

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[11]In that respect we fully agree with Ref. [23].

[12]A "test particle" must have negligible size as compared to the curvature radius of the background geometry, so as to not couple to second and higher derivatives of the metric (i.e., no curvature couplings). At the same time, it cannot be too small, so as to not create a significant gravitational self-energy and an appreciable self-gravitational field on top of that of background spacetime. Moreover, it may have no nonvanishing charges, spin, or higher moments amongst its mass multipoles. This should make it clear that the notion of "test particle" is contextual and approximative. One and the same object may be a good test particle in one situation and badly fail to be such in another.

radiation-reaction and also that we avoided obstructions on the applicability of the Hamiltonian formalism that result from the infamous "no-interaction theorem" [28], whose impact only starts at the sixth order in a c^{-1} expansion [29].

As for Ref. [1] in the gravity-free case, we see the virtue of our calculation in its firm rooting in explicitly spelled out principles, which leave no doubt concerning the questions of consistency and completeness of 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 semiclassical notions, like smooth worldlines and comparisons of their associated lengths (i.e., "proper time" and "redshift"); see, e.g., Refs. [3–8]. We emphasized in the introduction and also in our discussion of the Equivalence Principle that answers to the fundamental question of gravity-matter coupling in Quantum Mechanics should not be based on *a priori* restricted states that imply a semiclassical behavior of some of the (factorizing) degrees of freedom. Rather, they should apply to all states in an equally valid fashion.

Similar to the gravity-free case, we now *derived* the result that the center 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 semiclassical grounds, but, as seen, its proper derivation requires some effort. We stress once more that for this interpretation it was crucial to express the Hamiltonian in terms of the physical spacetime metric. As a result, our work lends 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; see, e.g., Refs. [3–8]. Moreover, it also applies to new experimental setups, like that of an ion trap in a gravitational field, currently under investigation [30] in extension of Ref. [31]. Finally we mention that due to our explicit parametrization of the gravitational field by means of the Eddington-Robertson parameters, our formulas will also apply to possible quantum tests of General Relativity against test theories within that class.

ACKNOWLEDGMENTS

APPENDIX: FORMULAS FROM THE PAPER OF SONNLEITNER AND BARNETT

In this Appendix we reproduce all formulas from Ref. [1] that are used in the main text, while providing a little context.

We use the original numbering, prepended with "A[1]." For formulas containing an error in Ref. [1], we give here a corrected version and the number is marked with an asterisk.

The classical Lagrangian for two particles interacting with electromagnetic potentials[13] is

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

Note that here, in the notation of Ref. [1], ϕ_{tot} is the total electric potential, not to be confused with our gravitational potential ϕ from the main text.

One then splits the electromagnetic potentials into internal (generated by the particles) and external parts, employs the Coulomb gauge and solves the Maxwell equations for the internal part in lowest order [see (A[1].A1) and (A[1].A3)]. Inserting the internal potential solutions and expanding the kinetic terms for the particles, one arrives at the post-Newtonian Lagrangian

$$L(\mathbf{r}_1, \dot{\mathbf{r}}_1, \mathbf{r}_2, \dot{\mathbf{r}}_2, \mathbf{A}^\perp, \dot{\mathbf{A}}^\perp)$$
$$= L_{\text{Darwin}}(\mathbf{r}_1, \dot{\mathbf{r}}_1, \mathbf{r}_2, \dot{\mathbf{r}}_2) + \frac{\varepsilon_0}{2} \int d^3\mathbf{x}\, [(\partial_t \mathbf{A}^\perp)^2$$
$$- c^2 (\nabla \times \mathbf{A}^\perp)^2] + \int d^3\mathbf{x}\, \mathbf{j} \cdot \mathbf{A}^\perp, \tag{A[1].8}$$

$$L_{\text{Darwin}}(\mathbf{r}_1, \dot{\mathbf{r}}_1, \mathbf{r}_2, \dot{\mathbf{r}}_2)$$
$$= \frac{m_1 \dot{\mathbf{r}}_1^2}{2} + \frac{m_1 \dot{\mathbf{r}}_1^4}{8c^2} + \frac{m_2 \dot{\mathbf{r}}_2^2}{2} + \frac{m_2 \dot{\mathbf{r}}_2^4}{8c^2}$$
$$- \frac{1}{4\pi\varepsilon_0} \frac{e_1 e_2}{r} \left(1 - \frac{\dot{\mathbf{r}}_1 \cdot \dot{\mathbf{r}}_2}{2c^2}\right) + \frac{e_1 e_2}{4\pi\varepsilon_0} \frac{(\dot{\mathbf{r}}_1 \cdot \mathbf{r})(\dot{\mathbf{r}}_2 \cdot \mathbf{r})}{2r^3 c^2}, \tag{A[1].9}$$

where $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and $r = |\mathbf{r}|$.

The classical Hamiltonian obtained by Legendre transforming this Lagrangian is

$$H = \frac{\bar{\mathbf{p}}_1^2}{2m_1} - \frac{\bar{\mathbf{p}}_1^4}{8m_1^3 c^2} + \frac{\bar{\mathbf{p}}_2^2}{2m_2} - \frac{\bar{\mathbf{p}}_2^4}{8m_2^3 c^2}$$
$$+ \frac{1}{4\pi\varepsilon_0} \frac{e_1 e_2}{r} \left(1 - \frac{\bar{\mathbf{p}}_1 \cdot \bar{\mathbf{p}}_2}{2m_1 m_2 c^2}\right) - \frac{e_1 e_2}{4\pi\varepsilon_0} \frac{(\bar{\mathbf{p}}_1 \cdot \mathbf{r})(\bar{\mathbf{p}}_2 \cdot \mathbf{r})}{2r^3 c^2 m_1 m_2}$$
$$+ \frac{\varepsilon_0}{2} \int d^3\mathbf{x}\, [(\mathbf{\Pi}^\perp/\varepsilon_0)^2 + c^2 (\nabla \times \mathbf{A}^\perp)^2], \tag{A[1].12*}$$

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

The PZW transformation operator is

$$U = \mathrm{e}^{-i\Lambda} = \exp\left[-\frac{i}{\hbar} \int d^3\mathbf{x}\, \boldsymbol{\mathcal{P}}(\mathbf{x}, t) \cdot \mathbf{A}^\perp(\mathbf{x}, t)\right], \tag{A[1].14*}$$

---

[13]In the absence of gravity, as this is the situation considered in Ref. [1].

where $\mathcal{P}$ is the polarization field

$$
\mathcal{P}(\mathbf{x}, t) = \sum_{i=1,2} e_i [\mathbf{r}_i(t) - \mathbf{R}(t)] \int_0^1 d\lambda\, \delta\{\mathbf{x} - \mathbf{R}(t)
$$
$$
- \lambda[\mathbf{r}_i(t) - \mathbf{R}(t)]\}. \qquad (\text{A[1].15})
$$

The transformation amounts to the following change of canonical momenta:

$$
\mathbf{p}_i \to U\mathbf{p}_i U^\dagger = \mathbf{p}_i + \hbar\nabla_{\mathbf{r}_i}\Lambda, \qquad (\text{A[1].19a})
$$

$$
\mathbf{\Pi}^\perp(\mathbf{x}) \to \mathbf{\Pi}^\perp(\mathbf{x}) + \mathcal{P}^\perp(\mathbf{x}). \qquad (\text{A[1].19b*})
$$

In electric dipole approximation, i.e., expanding to first order in $\bar{\mathbf{r}}_i := \mathbf{r}_i - \mathbf{R}$, and using $\sum_{j=1,2} e_j = 0$, we find

$$
\hbar\nabla_{\mathbf{r}_{1,2}}\Lambda \simeq e_{1,2}[\mathbf{A}^\perp(\mathbf{R}) + (\bar{\mathbf{r}}_{1,2}\cdot\nabla)\mathbf{A}^\perp(\mathbf{R})]
$$
$$
+ \frac{e_1\mathbf{r}_1 + e_2\mathbf{r}_2}{2}\times[\nabla\times\mathbf{A}^\perp(\mathbf{R})]. \qquad (\text{A[1].21*})
$$

Thus, under the PZW transformation and the dipole approximation the momenta transform as $\mathbf{p}_i - e_i\mathbf{A}(\mathbf{r}_i) \to \mathbf{p}_i + \mathbf{d}\times\mathbf{B}(\mathbf{R})/2$ (*), where $\mathbf{d}$ is the dipole moment.

Terms of the form

$$
\frac{\mathbf{p}_i\cdot[\mathbf{d}\times\mathbf{B}(\mathbf{R})]}{m_i m_j c^2} \propto \frac{|\mathbf{p}_i|}{m_i c}\frac{|\mathbf{d}\cdot\mathbf{E}(\mathbf{R})|}{m_j c^2} \qquad (\text{A[1].22})
$$

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 particles. The multipolar Hamiltonian in electric dipole approximation is then

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

where $\mathcal{P}_d = +\mathbf{d}\delta(\mathbf{x} - \mathbf{R})$ (*) is the polarization in electric dipole approximation.

Expressed in Newtonian center of mass coordinates, the Hamiltonian is as follows:

$$
H_{[\text{com}]} = H_C + H_A + H_{AL} + H_L + H_X, \qquad (\text{A[1].25a})
$$

$$
H_C = \frac{\mathbf{P}^2}{2M}\left[1 - \frac{\mathbf{P}^2}{4M^2 c^2} - \frac{1}{Mc^2}\left(\frac{\mathbf{p}_r^2}{2\mu} - \frac{e^2}{4\pi\varepsilon_0 r}\right)\right], \qquad (\text{A[1].25b*})
$$

$$
H_A = \frac{\mathbf{p}_r^2}{2\mu}\left(1 - \frac{m_1^3 + m_2^3}{M^3}\frac{\mathbf{p}_r^2}{4\mu^2 c^2}\right) - \frac{e^2}{4\pi\varepsilon_0}
$$
$$
\times\left[\frac{1}{r} + \frac{1}{2\mu M c^2}\left(\mathbf{p}_r\cdot\frac{1}{r}\mathbf{p}_r + \mathbf{p}_r\cdot\mathbf{r}\frac{1}{r^3}\mathbf{r}\cdot\mathbf{p}_r\right)\right], \qquad (\text{A[1].25c})
$$

$$
H_{AL} = -\mathbf{d}\cdot\mathbf{E}^\perp(\mathbf{R}) + \frac{1}{2M}\{\mathbf{P}\cdot[\mathbf{d}\times\mathbf{B}(\mathbf{R})] + \text{H.c.}\}
$$
$$
- \frac{m_1 - m_2}{4m_1 m_2}\{\mathbf{p}_r\cdot[\mathbf{d}\times\mathbf{B}(\mathbf{R})] + \text{H.c.}\}
$$
$$
+ \frac{1}{8\mu}(\mathbf{d}\times\mathbf{B}(\mathbf{R}))^2 + \frac{1}{2\varepsilon_0}\int d^3\mathbf{x}\,\mathcal{P}_d^{\perp 2}(\mathbf{x}, t),
$$
$$
(\text{A[1].25d*})
$$

$$
H_L = \frac{\varepsilon_0}{2}\int d^3\mathbf{x}\,(\mathbf{E}^{\perp 2} + c^2\mathbf{B}^2), \qquad (\text{A[1].25e})
$$

$$
H_X = -\frac{(\mathbf{P}\cdot\mathbf{p}_r)^2}{2M^2\mu c^2} + \frac{e^2}{4\pi\varepsilon_0 r}\frac{(\mathbf{P}\cdot\mathbf{r}/r)^2}{2M^2 c^2}
$$
$$
+ \frac{m_1 - m_2}{2\mu M^2 c^2}\left\{(\mathbf{P}\cdot\mathbf{p}_r)\mathbf{p}_r^2/\mu - \frac{e^2}{8\pi\varepsilon_0}\right.
$$
$$
\left.\times\left[\frac{1}{r}\mathbf{P}\cdot\mathbf{p}_r + \frac{1}{r^3}(\mathbf{P}\cdot\mathbf{r})(\mathbf{r}\cdot\mathbf{p}_r) + \text{H.c.}\right]\right\}. \qquad (\text{A[1].25f})
$$

The canonical transformation into new coordinates $\mathbf{Q}$, $\mathbf{q}$, $\mathbf{p}$ used to eliminate the cross terms H_X reads as follows:

$$
\mathbf{R} = \mathbf{Q} + \frac{m_1 - m_2}{2M^2 c^2}\left[\left(\frac{\mathbf{p}^2}{2\mu}\mathbf{q} + \text{H.c.}\right) - \frac{e^2}{4\pi\varepsilon_0 q}\mathbf{q}\right]
$$
$$
- \frac{1}{4M^2 c^2}[(\mathbf{q}\cdot\mathbf{P})\mathbf{p} + (\mathbf{P}\cdot\mathbf{p})\mathbf{q} + \text{H.c.}], \qquad (\text{A[1].26a})
$$

$$
\mathbf{r} = \mathbf{q} + \frac{m_1 - m_2}{2\mu M^2 c^2}[(\mathbf{q}\cdot\mathbf{P})\mathbf{p} + \text{H.c.}] - \frac{\mathbf{q}\cdot\mathbf{P}}{2M^2 c^2}\mathbf{P}, \quad (\text{A[1].26b})
$$

$$
\mathbf{p}_r = \mathbf{p} + \frac{\mathbf{p}\cdot\mathbf{P}}{2M^2 c^2}\mathbf{P} - \frac{m_1 - m_2}{2M^2 c^2}
$$
$$
\times\left\{\frac{\mathbf{p}^2}{\mu}\mathbf{P} - \frac{e^2}{4\pi\varepsilon_0}\left[\frac{1}{q}\mathbf{P} - \frac{1}{q^3}(\mathbf{P}\cdot\mathbf{q})\mathbf{q}\right]\right\}. \qquad (\text{A[1].26c})
$$

The internal electromagnetic potentials up to our order of approximation (thus neglecting retardation) are as follows:

$$
\phi_{\text{el.,ng}}(\mathbf{x}, t) = \frac{1}{4\pi\varepsilon_0}\int d^3\mathbf{x}'\frac{\rho(\mathbf{x}', t)}{|\mathbf{x} - \mathbf{x}'|}, \qquad (\text{A[1].A1})
$$

$$
\mathcal{A}_{\text{ng}}^\perp(\mathbf{x}, t) \simeq \frac{\mu_0}{4\pi}\int d^3\mathbf{x}'\frac{\mathbf{j}(\mathbf{x}', t)}{|\mathbf{x} - \mathbf{x}'|} + \frac{\mu_0}{(4\pi)^2}\int d^3\mathbf{x}'
$$
$$
\times\int d^3\mathbf{x}''\frac{\mathbf{x} - \mathbf{x}'}{|\mathbf{x} - \mathbf{x}'|^3}\frac{\mathbf{j}(\mathbf{x}'', t)\cdot(\mathbf{x}' - \mathbf{x}'')}{|\mathbf{x}' - \mathbf{x}''|^3}
$$
$$
= \frac{\mu_0}{8\pi}\sum_{i=1,2}e_i\left\{\frac{\dot{\mathbf{r}}_i}{|\mathbf{x} - \mathbf{r}_i|} + \frac{(\mathbf{x} - \mathbf{r}_i)[\dot{\mathbf{r}}_i\cdot(\mathbf{x} - \mathbf{r}_i)]}{|\mathbf{x} - \mathbf{r}_i|^3}\right\}.
$$
$$
(\text{A[1].A3})
$$

Here we have changed the variable names of the potentials to conform to our notation; in particular we added the suffix "ng," standing for "nongravitational."

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