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One-electron atom as a probe of spacetime curvature

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We consider a one-electron atom in an arbitrary curved spacetime. After reviewing the generalization of the Dirac equation to curved spacetime, we develop the perturbation theory of degenerate stationary states taking into account the Hermiticity properties appropriate to curved spacetime. We then calculate the Hamiltonian of the Dirac equation in Fermi normal coordinates to first order in the Riemann tensor, including the corrections to the electromagnetic field. As an application of these results, we obtain expressions in terms of the Riemann tensor for the shifts produced by the local curvature in the nonrelativistic $1S$, $2S$, and $2P$ energy levels, and in the relativistic $1S_{1/2}$, $2S_{1/2}$, and $2P_{1/2}$ energy levels.

I. INTRODUCTION

The energy levels of an atom will be shifted when the atom is placed in a region of curved spacetime. The energies of the various levels will be altered in different ways, so that the effect of curvature can be distinguished from other effects, and the atomic spectrum can in principle be used to measure or put an upper limit on the curvature of spacetime at the position of the atom. For that purpose, one requires expressions for the energy-level shifts as a function of the local Riemann curvature tensor in an arbitrary curved spacetime (we do not consider nontrivial topologies or twisted fields).

Although the hydrogen atom has been studied in particular curved spacetimes, there are contradictory conclusions in the literature, and to our knowledge no one has given explicit expressions for energy-level shifts, as we do here. References and a critique of the previous literature are given by Audretsch and Schäfer,[1] who considered the hydrogen atom in certain cosmological metrics. The problem of finding the perturbations of the energy levels of an atom placed in a curved spacetime is of considerable theoretical interest, as well as possible observational interest.[2]

We find that for the perturbation of the energy levels of hydrogen to be as large as the Lamb shift (4.4×10^{-6} eV), the required characteristic radius of curvature, D, of the spacetime would have to be as small as 10^{-3} cm. Although the existence of accessible regions of such large curvature may seem unlikely from the viewpoint of the general theory of relativity, it is nevertheless of interest to have a measuring instrument which can objectively test for regions of large curvature which may be at large distances from us. The atom and its spectrum provides such an instrument.

We first review the formalism of the Dirac equation generalized to curved spacetime, and set up the necessary perturbation theory. Then we calculate the curvature-induced energy-level shifts for the relativistic $1S_{1/2}$, $2S_{1/2}$, and $2P_{1/2}$ states, working to first order in the Riemann curvature tensor. The Hamiltonian given here can be used to calculate the shifts of any energy levels, as well as other effects. For the $1S_{1/2}$ levels, we work to all orders in the fine-structure constant, while for the $2S_{1/2}$ and $2P_{1/2}$ levels our results are valid to lowest order in the fine-structure constant. The nonrelativistic limit of the theory is also discussed, and the shifts of the $1S$, $2S$, and $2P$ levels are calculated.

We make use of coordinates which are locally inertial (normal) at the position of the atom. In particular, we use Fermi normal coordinates because they are normal along the entire spacetime path of the freely falling atom, and thus seem appropriate (in view of the time-energy uncertainty relation) for a problem involving energy levels. The metric is expressed in terms of the value of the curvature tensor at the center of mass of the atom. That value is assumed to be slowly changing on time scales of the order associated with the atomic processes under study.

Differences between the calculated energy levels correspond to the frequencies of the emitted radiation as measured by a detector placed near the atom and at rest with respect to it (or more precisely by a hypothetical detector at the center of mass of the atom). The frequencies observed far from the atom will have additional Doppler, cosmological, and gravitational shifts. These latter shifts are the same for all spectral lines. They can be determined by observation of a small number of lines and subtracted away. The remaining shifts can then be compared with the calculated expressions for the shifts as a function of the Riemann tensor at the position of the atom.

We assume (i) that a metric description of space-

time is valid, (ii) that the Dirac equation generalized to curved spacetime governs the system, (iii) that, to good approximation, the atom is in free fall along a geodesic of the spacetime during the time required for an atomic transition, and (iv) that the time rate of change of the Riemann tensor as measured along the spacetime path of the atom is sufficiently small on an atomic time scale that well-defined energy levels exist. The third assumption is plausible because the motion of the atom as a whole is mainly governed by the nucleus, and for the range of curvatures under consideration the external Riemann tensor does not change significantly over the dimensions of the nucleus.

In Secs. II and III we review the formalism of the Dirac equation in curved spacetime and define the conserved scalar product for the Hilbert space of one-electron states. In Sec. IV, we discuss the Hermiticity of the Hamiltonian with respect to the scalar product. In Sec. V, we develop the perturbation theory of degenerate energy levels. In Secs. VI, VII, and VIII, the Hamiltonian of the Dirac equation for the one-electron atom is obtained in Fermi normal coordinates, including all terms of first order in the Riemann curvature tensor (the calculation of the electromagnetic field to that order is given in Sec. VII). The nonrelativistic limit is considered in Sec. IX, and the perturbations of the $1S$, $2S$, and $2P$ levels are found. The relativistic $1S_{1/2}$, $2S_{1/2}$, and $2P_{1/2}$ levels are discussed in Sec. X and XI. Finally, the results are summarized and put in generally covariant form in Sec. XII.

II. DIRAC EQUATION IN CURVED SPACETIME

To write the Dirac equation in a curved spacetime of metric $g_{\mu\nu}$, one introduces coordinate-dependent matrices $\underline{\gamma}^{\mu}(x)$, which satisfy the equation[3,4,5]

$$\underline{\gamma}^{\mu}(x)\underline{\gamma}^{\nu}(x)+\underline{\gamma}^{\nu}(x)\underline{\gamma}^{\mu}(x)=2g^{\mu\nu}(x)\,. \tag{2.1}$$

One also introduces spinorial affine connections $\Gamma_{\mu}(x)$, which are matrices defined by the vanishing of the covariant derivative of the $\underline{\gamma}$ matrices:

$$\nabla_{\mu}\underline{\gamma}_{\nu}\equiv\partial_{\mu}\underline{\gamma}_{\nu}-\Gamma^{\lambda}_{\mu\nu}\underline{\gamma}_{\lambda}-\Gamma_{\mu}\underline{\gamma}_{\nu}+\underline{\gamma}_{\nu}\Gamma_{\mu}=0\,, \tag{2.2}$$

where the indices on $\underline{\gamma}^{\mu}$ have been lowered with the metric tensor. The covariant derivative acting on a spinor field ψ is then

$$\nabla_{\mu}\psi=(\partial_{\mu}-\Gamma_{\mu})\psi\,, \tag{2.3}$$

and the generally covariant form of the Dirac equation is

$$[\underline{\gamma}^{\mu}(x)\nabla_{\mu}+m]\psi(x)=0\,, \tag{2.4}$$

where m is the mass.

For the purpose of defining a conserved probability current density S^{μ} which transforms as a four-vector, Bargmann (Ref. 4) defines a matrix $\epsilon(x)$ by means of the following conditions:

$$\epsilon+\epsilon^{\dagger}=0\,, \tag{2.5}$$

$$\epsilon\underline{\gamma}^{\mu}+\underline{\gamma}^{\mu\dagger}\epsilon=0\,, \tag{2.6}$$

$$\nabla_{\mu}\epsilon\equiv\partial_{\mu}\epsilon+\Gamma^{\dagger}_{\mu}\epsilon+\epsilon\Gamma_{\mu}=0\,. \tag{2.7}$$

Then the probability current density

$$S^{\mu}\equiv-\psi^{\dagger}\epsilon\underline{\gamma}^{\mu}\psi \tag{2.8}$$

can be shown to transform as a four-vector under general coordinate transformations, and to satisfy the conservation equation

$$\nabla_{\mu}S^{\mu}=0\,. \tag{2.9}$$

Define a vierbein field $b^{\alpha}{}_{\mu}(x)$ such that

$$g_{\mu\nu}(x)=\eta_{\alpha\beta}b^{\alpha}{}_{\mu}(x)b^{\beta}{}_{\nu}(x)\,, \tag{2.10}$$

where $\eta_{\alpha\beta}$ is the flat-spacetime metric tensor with $\eta_{00}=-1$, $\eta_{11}=\eta_{22}=\eta_{33}=1$. Under transformations of the coordinates, indices $\mu,\nu,\lambda,\ldots$ are regarded as tensor indices, while indices $\alpha,\beta,\ldots$ act merely as labels (thus the $b^{\alpha}{}_{\mu}$ constitute four different vector fields). In addition to the covariance of the formalism under general coordinate transformations acting on the spacetime indices μ,ν, the formalism is also covariant under Lorentz transformations applied to the vierbein indices α, β. Under such Lorentz transformation, the $\underline{\gamma}^{\mu}$ are invariant, while the ψ transform as in special relativity forming a spinor representation of the Lorentz group. On the other hand, under coordinate transformations one can regard ψ as invariant (or alternatively, as undergoing an arbitrary matrix transformation, with a corresponding matrix transformation also applied to the $\underline{\gamma}^{\mu}$, in addition to the tensor transformation of the index μ). Vierbein indices are lowered with $\eta_{\alpha\beta}$, while spacetime indices are lowered with the metric $g_{\mu\nu}$. Also introduce the constant special-relativistic matrices γ_{α}, defined by

$$\gamma_{\alpha}\gamma_{\beta}+\gamma_{\beta}\gamma_{\alpha}=2\eta_{\alpha\beta}\,. \tag{2.11}$$

These matrices can be chosen such that

$$\gamma_0^{\dagger}=-\gamma_0\,,\quad \gamma_i^{\dagger}=\gamma_i\quad(i=1,2,3)\,. \tag{2.12}$$

It follows from Eqs. (2.1), (2.10), and (2.11) that

$$\underline{\gamma}_{\mu}(x)=b^{\alpha}{}_{\mu}(x)\gamma_{\alpha}\,. \tag{2.13}$$

Expressed in terms of the vierbein and the constant γ matrices, the solution of Eq. (2.2) is

$$\Gamma_{\mu}=-\tfrac{1}{4}\gamma_{\alpha}\gamma_{\beta}b^{\alpha}{}_{\nu}g^{\nu\lambda}\nabla_{\mu}b^{\beta}{}_{\lambda}+iqA_{\mu}1\,, \tag{2.14}$$

where

$$\nabla_{\mu}b^{\beta}{}_{\lambda}=\partial_{\mu}b^{\beta}{}_{\lambda}-\Gamma^{\sigma}{}_{\mu\lambda}b^{\beta}{}_{\sigma}\,. \tag{2.15}$$

The second term on the right-hand side of Eq. (2.14), which is proportional to the unit matrix, is not determined by Eq. (2.2). However, it is clear from Eqs. (2.3) and (2.4) that the constant q may be interpreted as the charge of the particle described by ψ, and the vector field A_μ as the vector potential of the electromagnetic field acting on the particles (we thus take q and A_μ to be real).

The matrix ϵ appearing in Eqs. (2.5)–(2.8) can be taken such that

$$\epsilon = \gamma^0 , \tag{2.16}$$

where $\gamma^0 = \eta^{0\alpha}\gamma_\alpha = -\gamma_0$. We prove this as follows. Clearly, Eq. (2.5) is satisfied by the above choice of ϵ. Also one has

$$\gamma^0\underline{\gamma}^\mu + \underline{\gamma}^{\mu\dagger}\gamma^0 = -g^{\mu\lambda}b^\alpha{}_\lambda(\gamma_0\gamma_\alpha + \gamma_\alpha^\dagger\gamma_0) = 0 , \tag{2.17}$$

as a consequence of Eqs. (2.11) and (2.12). Thus, Eq. (2.6) is satisfied. Finally, the left side of Eq. (2.7) becomes, with the present choice of ϵ,

$$\nabla_\mu\epsilon = \tfrac{1}{4}b^\alpha{}_\nu g^{\nu\lambda}\nabla_\mu b^\beta{}_\lambda(\gamma_\beta^\dagger\gamma_\alpha^\dagger\gamma_0 + \gamma_0\gamma_\alpha\gamma_\beta) .$$

But using $\gamma_\alpha^\dagger\gamma_0 = -\gamma_0\gamma_\alpha$ and Eq. (2.11), one finds that

$$\gamma_\beta^\dagger\gamma_\alpha^\dagger\gamma_0 + \gamma_0\gamma_\alpha\gamma_\beta = 2\gamma_0\eta_{\alpha\beta} .$$

Hence

$$\nabla_\mu\epsilon = \tfrac{1}{2}\gamma_0\eta_{\alpha\beta}b^\alpha{}_\nu g^{\mu\lambda}\nabla_\mu b^\beta{}_\lambda = 0 ,$$

which proves that Eq. (2.7) is satisfied. The last quantity vanishes because $\eta_{\alpha\beta}$ is symmetric, while $b^\alpha{}_\nu g^{\nu\lambda}\nabla_\mu b^\beta{}_\lambda$ is antisymmetric in α,β. (The latter follows from $\eta^{\alpha\beta} = b^\alpha{}_\nu g^{\nu\lambda}b^\beta{}_\lambda$, and $\nabla_\mu\eta^{\alpha\beta} = \partial_\mu\eta^{\alpha\beta} = 0$ because $\eta^{\alpha\beta}$ is a scalar under spacetime coordinate transformations.) The choice $\epsilon = \gamma^0$ of Eq. (2.16) is invariant under coordinate transformations, and we will work with a vierbein such that Eq. (2.16) holds.

III. SCALAR PRODUCT AND HILBERT SPACE

Let us define the scalar product

$$(\phi,\psi) \equiv -\int d^3x\sqrt{-g}\,\phi^\dagger\gamma^0\underline{\gamma}^0(x)\psi , \tag{3.1}$$

where the integration is over a constant x^0 Cauchy hypersurface. This scalar product is linear in ψ and antilinear in ϕ. If ϕ and ψ satisfy Eq. (2.4), then

$$\frac{d}{dt}(\phi,\psi) = 0 , \tag{3.2}$$

where $t = x^0$. This follows from

$$\nabla_\mu(\phi^\dagger\gamma^0\underline{\gamma}^\mu\psi) = 0 , \tag{3.3}$$

where we used Eq. (2.4) and its adjoint, as well as Eqs. (2.17), (2.7), and (2.2) (we assume throughout that ϕ,ψ vanish sufficiently rapidly at spatial infinity or obey suitable boundary conditions in a closed universe, so that the spatial components of (3.3) give vanishing contributions upon integration and the various products are well defined).

One readily finds, as a consequence of Eqs. (2.12) and (2.17), that

$$(\phi,\psi)^* = (\psi,\phi) , \tag{3.4}$$

where the asterisk denotes complex conjugation. Thus (ψ,ψ) is real. We show it is positive definite as follows. One has

$$(\psi,\psi) = \int d^3x\sqrt{-g}\,S^0 , \tag{3.5}$$

where S^μ is the four-vector defined in Eq. (2.8). At an arbitrary given point x, one can choose a locally inertial coordinate system such that $\underline{\gamma}^\mu(x) = \gamma^\mu$ at the given point, so that $S^0(x) = \psi^\dagger(x)\psi(x)$ is positive definite. As in special relativity it follows that $S^\mu(x)$ is a timelike vector lying in the forward light cone. The general coordinate transformations under consideration are required to preserve the direction of time and to preserve the timelike or spacelike character of vectors. Hence in the general coordinates x^μ, it follows that S^μ is timelike with S^0 positive definite at all points. Therefore, (ψ,ψ) of Eq. (3.5) is positive definite, vanishing if and only if ψ vanishes.

The above properties of the scalar product (ϕ,ψ) imply that the spinors ψ with (ψ,ψ) finite form a Hilbert space, which we take as the space of states of the system. We call (ϕ,ψ) of Eq. (3.1) the curved scalar product, in contrast to the flat scalar product $(\phi,\psi)_0$ defined by

$$(\phi,\psi)_0 = \int d^3x\,\phi^\dagger\psi . \tag{3.6}$$

This latter scalar product is not appropriate to the Hilbert space of physical states because it is not conserved when ψ and ϕ satisfy the Dirac equation in curved spacetime, and the formalism based on it would not be generally covariant. One may base the usual probability interpretation of this quantum-mechanical system on the curved scalar product (ϕ,ψ), but not on the flat scalar product $(\phi,\psi)_0$.

IV. THE HAMILTONIAN AND ITS HERMITICITY

Multiplying Eq. (2.4) on the left by $\underline{\gamma}^0(x)$ and dividing by $g^{00}(x)$ allows us to write the Dirac equation in the form

$$i\partial_0\psi = H\psi , \tag{4.1}$$

with the Hamiltonian

$$H = -i(g^{00})^{-1}\underline{\gamma}^0\underline{\gamma}^i(\partial_i - \Gamma_i) + i\Gamma_0 - i(g^{00})^{-1}\underline{\gamma}^0 m , \tag{4.2}$$

where repeated Latin indices are summed from 1 to 3. The vanishing of $d(\psi,\psi)/dt$ implies that

$$(\psi, H\psi) - (H\psi, \psi) = i \int d^3x\, \psi^\dagger \gamma^0 \frac{\partial}{\partial t} (\sqrt{-g}\, \underline{\gamma}^0)\psi . \tag{4.3}$$

Thus, in general H will not be Hermitian with respect to the conserved scalar product (nor with respect to the flat scalar product). This may reflect the fact that in the presence of a time-changing gravitational field the single-particle sector of the Hilbert space of the many-particle theory is not self-contained, as the number of particles present can change. However, we will not dwell on that question, as our interest here is in the stationary states of a one-electron atom. For stationary-state solutions of Eq. (4.1) to exist in a locally inertial rest frame of the atom, we must treat the time dependence of the Riemann tensor in such a frame of reference as adiabatic (slow), in accordance with assumption (iv) of Sec. I. This implies that in the region where the probability of finding the electron is significant, the quantity $\partial(\sqrt{-g}\,\underline{\gamma}^0)/\partial t$ is sufficiently small that the right side of Eq. (4.3) can be neglected (as can be seen directly from the explicit expressions for $g_{\mu\nu}$ and $\underline{\gamma}^0$ given later). Then

$$(\psi, H\psi) = (H\psi, \psi) , \tag{4.4}$$

and one can regard H as Hermitian with respect to the curved scalar product [for a stationary metric Eq. (4.4) is exact].

It follows in the standard way (but using the curved scalar product) that the eigenvalues E of H are real, and that eigenfunctions ψ_1, ψ_2 belonging to different eigenvalues E_1, E_2 are orthogonal with respect to the curved scalar product. We interpret H as the observable corresponding to the energy in a locally inertial rest frame of the atom.

V. DEGENERATE-STATIONARY-STATE PERTURBATION THEORY

The Dirac Hamiltonian in flat spacetime is

$$H_0 = i\gamma^0\gamma^i(\partial_i - iqA_i^{(0)}) - qA_0^{(0)} + i\gamma^0 m. \tag{5.1}$$

Let us suppose that the operator

$$H_I \equiv H - H_0 \tag{5.2}$$

can be regarded as small. Here H is the Hamiltonian of Eq. (4.2), which includes the electromagnetic field A_μ through the Γ_μ of Eq. (2.14). The application of perturbation theory to the problem of finding the eigenvalue of H is complicated by the fact that H_I is not, in general, Hermitian with respect to either the curved or flat scalar product. That is because H_0 is Hermitian only with respect to the flat scalar product of Eq. (3.6), while H is Hermitian only with respect to the curved scalar product of Eq. (3.1). Therefore, the orthonormality properties of their respective sets of eigenfunctions refer to different scalar products, and one must exercise caution. Nevertheless, one can carry out the perturbation theory almost as in flat spacetime.

Consider an eigenvalue $E^{(0)}$ of H_0 which is n-fold degenerate. Then we can write

$$H_0\phi_a^{(0)} = E^{(0)}\phi_a^{(0)}, \quad a = 1, \ldots, n \tag{5.3}$$

with

$$(\phi_a^{(0)}, \phi_b^{(0)})_0 = \delta_{ab} . \tag{5.4}$$

The n eigenfunctions $\phi_a^{(0)}$ span the space $\mathcal{H}_0$ of eigenfunctions of H_0 belonging to the eigenvalue $E^{(0)}$, and are orthonormal with respect to the flat scalar product. If we imagine curvature in the region of spacetime where the atom is located to be parametrized by a quantity λ, such that as λ approaches 0, the region of spacetime becomes flat, then there will exist n eigenvalues E_i of H which approach $E^{(0)}$ as λ vanishes. Thus, we can write

$$H\psi_i = E_i\psi_i, \quad i = 1, \ldots, n \tag{5.5}$$

with

$$(\psi_i, \psi_j) = 0 \quad \text{for } i \neq j . \tag{5.6}$$

The ψ_i are orthogonal with respect to the curved scalar product. Also, because H approaches H_0, each ψ_i will approach an eigenfunction $\psi_i^{(0)}$ of H_0 belonging to the space $\mathcal{H}_0$ as λ vanishes.

Assuming analyticity and working to first order in λ, we can write

$$H = H_0 + \lambda H_I , \tag{5.7}$$

$$\psi_i = \psi_i^{(0)} + \lambda\psi_i^{(1)} , \tag{5.8}$$

and

$$E_i = E^{(0)} + \lambda E_i^{(1)} , \tag{5.9}$$

where λH_I in Eq. (5.7) is the first term in the expansion of Eq. (5.2) in powers of λ (thus, it might more accurately be written as $\lambda H_I^{(1)}$). One can continue in the same way to higher orders in λ, but we will work to first order in the curvature here. It follows from Eq. (5.5) that

$$H_0\psi_i^{(0)} = E^{(0)}\psi_i^{(0)} , \tag{5.10}$$

and

$$H_I\psi_i^{(0)} + H_0\psi_i^{(1)} = E^{(0)}\psi_i^{(1)} + E_i^{(1)}\psi_i^{(0)} . \tag{5.11}$$

The $\psi_i^{(0)}$ lie in $\mathcal{H}_0$, as a consequence of Eq. (5.10), so that we can write

$$\psi_i^{(0)} = \sum_b \phi_b^{(0)}(\phi_b^{(0)}, \psi_i^{(0)})_0 . \tag{5.12}$$

Equation (5.11) implies that

$$(\phi_a^{(0)}, H_I\psi_i^{(0)})_0 + (\phi_a^{(0)}, H_0\psi_i^{(1)})_0 = E^{(0)}(\phi_a^{(0)}, \psi_i^{(1)})_0 + E_i^{(1)}(\phi_a^{(0)}, \psi_i^{(0)})_0 . \quad (5.13)$$

Using the Hermiticity of H_0 with respect to the flat scalar product and Eqs. (5.3), (5.12), and (5.4), one obtains

$$\sum_b [(\phi_a^{(0)}, H_I\phi_b^{(0)})_0 - E_i^{(1)}\delta_{ab}](\phi_b^{(0)}, \psi_i^{(0)})_0 = 0 . \quad (5.14)$$

Thus, the equation for the energy shifts $E_i^{(1)}$ is

$$\det[(\phi_a^{(0)}, H_I\phi_b^{(0)})_0 - E_i^{(1)}\delta_{ab}] = 0 . \quad (5.15)$$

That equation has the same form as in the usual perturbation theory of a degenerate energy eigenvalue. However, H_I is not Hermitian. The reality of $E_i^{(1)}$ is guaranteed by Eq. (5.9) because E and $E^{(0)}$ are each real, being eigenvalues of operators that are Hermitian with respect to the curved and flat scalar products, respectively. The diagonal matrix elements $(\phi_a^{(0)}, H_I\phi_a^{(0)})_0$ are also real, despite the fact that H_I is not Hermitian. That is a consequence of $\phi_a^{(0)}$ being an eigenfunction of H_0. One can write to first order in λ,

$$(\phi, \psi) = (\phi, \psi)_0 + \lambda(\phi, L\psi)_0 , \quad (5.16)$$

where λL arises in Eq. (3.1) from the first order term in the expansion of $\sqrt{-g}\underline{\gamma}^0(x)$ in powers of the curvature [the expansion is given explicitly in Eq. (8.18)]. Therefore, to first order in λ,

$$(\phi_a^{(0)}, H\phi_a^{(0)}) = E^{(0)}(\phi_a^{(0)}, \phi_a^{(0)}) + \lambda(\phi_a^{(0)}, H_I\phi_a^{(0)})_0 . \quad (5.17)$$

The left-hand side is real because H is Hermitian with respect to the curved scalar product, and the first term on the right-hand side is clearly real. Hence $(\phi_a^{(0)}, H_I\phi_a^{(0)})_0$ is real. We will use Eq. (5.15) to calculate to first order in the Riemann curvature tensor the perturbations of the relativistic $1S_{1/2}$, $2S_{1/2}$, and $2P_{1/2}$ energy levels, and of the nonrelativistic $1S$, $2S$, and $2P$ energy levels of a one-electron atom.

VI. METRIC AND AFFINITIES IN FERMI NORMAL COORDINATES

We assume that to good approximation the atom is falling along a geodesic G of the spacetime during the emission process. In Fermi normal coordinates,[6-8] each spacelike hypersurface of constant x^0 is normal to this geodesic and contains the set of spacelike geodesics normal to G. The time x^0 of an event in the hypersurface is the proper time along G at the point P where it intersects the hypersurface. The spatial coordinates x^i of an event occuring at time x^0 are given by $x^i = l(dx^i/dl)_P$, where l is the proper distance measured along the geodesic in the constant x^0 hypersurface which joins the event to point P. The metric in these coordinates to second order takes the form[7]

$$g_{00} = -1 - R_{0l0m}x^l x^m , \quad (6.1)$$

$$g_{0i} = g^{0i} = -\tfrac{2}{3}R_{0lim}x^l x^m , \quad (6.2)$$

$$g_{ij} = \delta_{ij} - \tfrac{1}{3}R_{iljm}x^l x^m , \quad (6.3)$$

$$g^{00} = -1 + R_{0l0m}x^l x^m , \quad (6.4)$$

$$g^{ij} = \delta^{ij} + \tfrac{1}{3}R^i{}_l{}^j{}_m x^l x^m , \quad (6.5)$$

$$g = -1 + \tfrac{1}{3}(R_{lm} - 2R_{0l0m})x^l x^m , \quad (6.6)$$

where Latin indices go from 1 to 3, and the Riemann tensor is evaluated at the point at which G intersects the constant x^0 hypersurface. Our sign conventions are those of Ref. 8, where $R^\alpha{}_{\beta\gamma\delta} = \partial_\gamma\Gamma^\alpha_{\beta\delta} - \cdots$. Eqs. (6.1)–(6.6) contain all terms linear in $R_{\alpha\beta\gamma\delta}$ (higher-order terms involve derivatives or products of $R_{\alpha\beta\gamma\delta}$). We find that the vierbein defined in Eq. (2.10) is

$$b^\alpha{}_0 = \delta^\alpha{}_0 - \tfrac{1}{2}R^\alpha{}_{l0m}x^l x^m , \quad (6.7)$$

$$b^\alpha{}_i = \delta^\alpha{}_i - \tfrac{1}{6}R^\alpha{}_{lim}x^l x^m , \quad (6.8)$$

and the affine connections are

$$\Gamma^0_{ij} = \tfrac{1}{3}(R_{0ijm} + R_{0jim})x^m , \quad \Gamma^0_{0i} = R_{0i0m}x^m ,$$
$$\Gamma^0_{00} = 0 , \quad \Gamma^i_{jk} = \tfrac{1}{3}(R_{jikm} + R_{kijm})x^m , \quad (6.9)$$
$$\Gamma^i_{0j} = R_{0mji}x^m , \quad \Gamma^i_{00} = R_{0i0m}x^m ,$$

where we are working to first order in $R_{\alpha\beta\gamma\delta}$. Using Eq. (2.14), the spinor affinities are found to be

$$\Gamma_0 = \tfrac{1}{2}\gamma_0\gamma_j R^j{}_{00m}x^m + \tfrac{1}{4}\gamma_k\gamma_j R^{kj}{}_{0m}x^m + iqA_0 , \quad (6.10)$$

and

$$\Gamma_i = \tfrac{1}{4}\gamma_0\gamma_j R^{0j}{}_{im}x^m + \tfrac{1}{8}\gamma_k\gamma_j R^{kj}{}_{im}x^m + iqA_i , \quad (6.11)$$

where indices are raised with the Minkowski metric $\eta^{\mu\nu}$. Here the γ_μ are the usual gamma matrices defined in Eq. (2.1), and A_μ is the electromagnetic vector potential.

VII. ELECTROMAGNETIC FIELD

Expressing the electromagnetic field in terms of a vector potential,

$$F_{\mu\nu} = \nabla_\mu A_\nu - \nabla_\nu A_\mu , \quad (7.1)$$

and imposing the Lorentz gauge condition

$$\nabla_\mu A^\mu = 0 , \tag{7.2}$$

one finds that the Maxwell equations are[8,9]

$$g^{\lambda\sigma}\nabla_\lambda\nabla_\sigma A_\mu - R_\mu{}^\nu A_\nu = -4\pi J_\mu , \tag{7.3}$$

where ∇_μ denotes the covariant derivative, and J_μ is the current vector (in Gaussian units). Using the expressions for the metric and affine connections given in Sec. VI, and working to first order in the Riemann tensor, we obtain for the Maxwell equations

$$\delta^{ij}\partial_i\partial_j A_0 + \tfrac{1}{3}R_{iljm}x^l x^m \partial^i\partial^j A_0 + \tfrac{5}{3}R_{i00m}x^m\partial^i A_0 + 2R^k{}_{i0m}x^m\partial^i A_k - \tfrac{2}{3}R^i{}_m x^m \partial_i A_0 = -4\pi J_0 , \tag{7.4}$$

and

$$\delta^{ij}\partial_i\partial_j A_k + \tfrac{1}{3}R_{iljm}x^l x^m\partial^i\partial^j A_k - \tfrac{2}{3}R^\nu{}_k A_\nu - \tfrac{1}{3}R^l{}_{00k}A_l + \tfrac{2}{3}\delta^{ij}(R^\alpha{}_{kim} + R^\alpha{}_{ikm})x^m\partial_j A_\alpha - \tfrac{1}{3}R^i{}_{00m}x^m\partial_i A_k - \tfrac{2}{3}R^i{}_m x^m\partial_i A_k = -4\pi J_k . \tag{7.5}$$

Time derivatives of A_μ have been neglected as being of higher order. That follows from our earlier assumption that derivatives of $R_{\alpha\beta\gamma\delta}$ are of higher order, as can be seen from the solution for the A_μ below. For a one-electron atom with a nuclear charge of Ze, one has

$$J_0 = -Ze\delta(\vec{r}), \quad J_k = 0 , \tag{7.6}$$

where $e = |e|$, and the minus sign arises from lowering the index on J^0 with the metric at $r = 0$. (Such effects as the finite size of the nucleus are regarded as perturbations which affect the energy additively and can be ignored in calculating the perturbation in the energy produced by the spacetime curvature.)

To lowest order the solution for A_μ is the Coulomb field. Thus,

$$A_0 = -Zer^{-1} + A_0^{(1)} \tag{7.7}$$

and

$$A_k = A_k^{(1)} , \tag{7.8}$$

where $A_\mu^{(1)}$ vanishes when $R_{\alpha\beta\gamma\delta}$ vanishes. To first order in $R_{\alpha\beta\gamma\delta}$, one has

$$\delta^{ij}\partial_i\partial_j A_0^{(1)} + \tfrac{1}{3}Zer^{-3}(3R^0{}_{l0m} - R_{lm})x^l x^m = 0 , \tag{7.9}$$

and

$$\delta^{ij}\partial_i\partial_j A_k^{(1)} + \tfrac{2}{3}ZeR^0{}_k r^{-1} + \tfrac{2}{3}ZeR^0{}_{lkm}x^l x^m r^{-3} = 0 . \tag{7.10}$$

We are working in normal coordinates, so that the deviation from the Coulomb field should vanish as one approaches the origin. Therefore, the appropriate boundary conditions are

$$A_0^{(1)} = 0, \quad A_k^{(0)} = 0 \text{ at } r = 0 . \tag{7.11}$$

The solutions are

$$A_0^{(1)} = \tfrac{1}{12}Ze(R + 4R_{00})r + \tfrac{1}{12}Ze(3R^0{}_{l0m} - R_{lm})x^l x^m r^{-1} , \tag{7.12}$$

and

$$A_k^{(1)} = \tfrac{1}{2}ZeR_{0k}r + \tfrac{1}{6}ZeR^0{}_{lkm}x^l x^m r^{-1} . \tag{7.13}$$

We note that the Lorentz-gauge condition of Eq. (7.2), to first order in the curvature, takes the form

$$\delta^{ij}\partial_i A_j^{(1)} = \tfrac{2}{3}ZeR_{0m}x^m r^{-1} , \tag{7.14}$$

which is satisfied by Eq. (7.13), as required for consistency.

VIII. DIRAC EQUATION AND HAMILTONIAN

In Sec. IV, we found that the generally covariant Dirac equation took the form

$$i\partial_0\psi = H\psi \tag{8.1}$$

with

$$H = -i(g^{00})^{-1}\underline{\gamma}^0\underline{\gamma}^i(\partial_i - \Gamma_i) + i\Gamma_0 - i(g^{00})^{-1}\underline{\gamma}^0 m , \tag{8.2}$$

where

$$\underline{\gamma}_\mu(x) = b^\alpha{}_\mu(x)\gamma_\alpha . \tag{8.3}$$

Let us write H to first order in $R_{\alpha\beta\gamma\delta}$ in Fermi normal coordinates.

Using Eqs. (6.4), (6.5), (7.7), (7.8), and (8.3), we obtain

$$-(g^{00})^{-1}\underline{\gamma}^0\underline{\gamma}^i = -\gamma_0\gamma_i - \tfrac{1}{6}R_{iljm}x^l x^m\gamma_0\gamma^j - \tfrac{1}{2}R_{0l0m}x^l x^m\gamma_0\gamma_i - \tfrac{1}{6}R_{0ljm}x^l x^m\gamma^j\gamma_i - \tfrac{1}{2}R_{0lim}x^l x^m , \tag{8.4}$$

where indices on the $\underline{\gamma}_\mu$ are raised with the spacetime metric, while indices on the γ_μ are raised with the Minkowski metric $(-1,1,1,1)$, and repeated Latin indices are summed from 1 to 3. In terms of the standard Dirac matrices $\vec{\alpha}$ and β, such that

$$\alpha_i\alpha_j+\alpha_j\alpha_i=2\delta_{ij},\quad \alpha_i\beta+\beta\alpha_i=0,\quad \beta^2=1, \tag{8.5}$$

one has

$$\gamma_0=i\beta \text{ and } \gamma_i=-i\beta\alpha_i. \tag{8.6}$$

Hence,

$$-(g^{00})^{-1}\underline{\gamma}^0\underline{\gamma}^i=-\alpha_i-\tfrac{1}{2}R_{0l0m}x^lx^m\alpha_i-\tfrac{1}{6}R_{iljm}x^lx^m\alpha^j-\tfrac{1}{6}R_{0ljm}x^lx^m\alpha^j\alpha_I-\tfrac{1}{2}R_{0lim}x^lx^m. \tag{8.7}$$

Then

$$H=-i\alpha^i\partial_i-\frac{i}{2}R_{0l0m}x^lx^m\alpha^i\partial_i-\frac{i}{6}R_{iljm}x^lx^m\alpha^j\partial^i-\frac{i}{6}R_{0ljm}x^lx^m\alpha^j\alpha^i\partial_i-\frac{i}{2}R_{0lim}x^lx^m\partial^i+i\alpha^i\Gamma_i+i\Gamma_0-i(g^{00})^{-1}\underline{\gamma}^0m, \tag{8.8}$$

where indices on α_i and ∂_i are raised with the Minkowski metric.

Using Eqs. (6.10) and (6.11), we obtain

$$i\alpha^i\Gamma_i+i\Gamma_0=\frac{i}{4}\alpha^j(R_{jm}-R_{0j0m})x^m+\frac{i}{4}\alpha^i\alpha^jR_{0imj}x^m-q\alpha^iA_i-qA_0. \tag{8.9}$$

The terms involving the electromagnetic vector potential are evaluated using Eqs. (7.7), (7.8), (7.12), and (7.13):

$$-q\alpha^iA_i-qA_0=-\zeta r^{-1}+\tfrac{1}{6}\zeta R_{0lmi}x^lx^m\alpha^ir^{-1}+\tfrac{1}{2}\zeta R_{0i}\alpha^ir-\tfrac{1}{12}\zeta(R_{lm}+3R_{0l0m})x^lx^mr^{-1}+\tfrac{1}{12}\zeta(R+4R_{00})r, \tag{8.10}$$

where we used $q=-e$, and defined the quantity

$$\zeta=Ze^2. \tag{8.11}$$

The last term in H is found to be

$$-i(g^{00})^{-1}\underline{\gamma}^0m=m\beta+\frac{m}{2}R_{0l0m}x^lx^m\beta-\tfrac{1}{6}mR_{il0m}x^lx^m\beta\alpha^i. \tag{8.12}$$

Finally, substituting these results in Eq. (8.8), we obtain

$$H=H_0+H_I, \tag{8.13}$$

with

$$H_0=-i\alpha^i\partial_i+m\beta-\zeta r^{-1}, \tag{8.14}$$

and

$$H_I=-\frac{i}{2}R_{0l0m}x^lx^m\alpha^i\partial_i-\frac{i}{6}R_{iljm}x^lx^m\alpha^j\partial^i-\frac{i}{6}R_{0ljm}x^lx^m\alpha^j\alpha^i\partial_i-\frac{i}{2}R_{0lim}x^lx^m\partial^i+\frac{i}{4}\alpha^j(R_{jm}-R_{0j0m})x^m+\frac{i}{4}\alpha^i\alpha^jR_{0imj}x^m+\tfrac{1}{6}\zeta R_{0lmi}x^lx^m\alpha^ir^{-1}+\tfrac{1}{2}\zeta R_{0i}\alpha^ir-\tfrac{1}{12}\zeta(R_{lm}+3R_{0l0m})x^lx^mr^{-1}+\tfrac{1}{12}\zeta(R+4R_{00})r+\tfrac{1}{2}mR_{0l0m}x^lx^m\beta-\tfrac{1}{6}mR_{il0m}x^lx^m\beta\alpha^i. \tag{8.15}$$

This includes all terms in H which are of first order in $R_{\alpha\beta\gamma\delta}$. Here the Riemann tensor is evaluated at the spatial origin of the Fermi normal coordinate system at time x^0, and is regarded as a slowly varying function of x^0.

The curved scalar product defined in Sec. III is

$$(\phi,\psi)=-\int d^3x\sqrt{-g}\,\phi^\dagger\gamma^0\underline{\gamma}^0\psi. \tag{8.16}$$

In Fermi normal coordinates to first order in the Riemann tensor, one has

$$(\phi,\psi)=(\phi,\psi)_0+(\phi,L\psi)_0, \tag{8.17}$$

where

$$L=-\tfrac{1}{6}(R_{lm}+R_{0l0m})x^lx^m-\tfrac{1}{6}R_{0lim}x^lx^m\alpha^i, \tag{8.18}$$

and

$$(\phi,\psi)_0=\int d^3x\,\phi^\dagger\psi \tag{8.19}$$

is the flat scalar product. We have checked by direct calculation, using Eqs. (8.13)–(8.15) and (8.17)–(8.19), that

$$(\phi,H\psi)=(H\phi,\psi), \tag{8.20}$$

so that H is Hermitian with respect to the curved scalar product. We therefore interpret H as the observable corresponding to the proper energy of the atom. To be more precise, we note that H generates the evolution of the state of the system from one spacelike hypersurface to the next in Fermi normal coordinates. These are the natural hypersurfaces of constant time for a hypothetical observer located at the nucleus (or center of mass) of the atom. The Fermi time coordinate corresponds essentially to the proper time of the nucleus (for the range of curvatures under consideration one can associate a proper time with the nucleus). Therefore, it is natural to interpret the difference between two energy levels of H as the energy of the photon emitted in the corresponding transition measured by a hypothetical detector located at the nucleus of the atom. (A detector located at the nucleus would have a finite probability of detecting the photon generated by an atomic

transition.) The values of the energy of such a photon as measured by a detector located outside the atom and by a detector located at the nucleus would evidently be related by the usual gravitational red (or blue) shift. It is in the above sense that we speak of H as corresponding to the proper energy of the atom, and of differences of the energy levels as corresponding to photon energies or frequencies measured by a detector located near the atom and at rest with respect to it.

Note that H is not Hermitian with respect to the flat scalar product. Also, H_0 is Hermitian only with respect to the flat scalar product, while H_I is not Hermitian with respect to either scalar product. The perturbation theory under these circumstances has been worked out to first order in the Riemann curvature tensor in Sec. V, with the result given in Eq. (5.15). We will use that expression to calculate the perturbations of the relativistic $1S_{1/2}$, $2S_{1/2}$, and $2P_{1/2}$ energy levels, including all terms in H_I which are linear in $R_{\alpha\beta\gamma\delta}$. However, first let us estimate the order of magnitude of the various terms in H_I [or more precisely, in $(\phi_a^{(0)}, H_I\phi_b^{(0)})_0$], and then find the nonrelativistic limit of the generally covariant Dirac equation. By the term "nonrelativistic limit" we mean, as usual, the limit in which the average velocity of the electron is small with respect to the speed of light, and not the limit of vanishing curvature.

IX. NONRELATIVISTIC LIMIT

The orders of magnitude of the matrix elements of the various terms in H_I are obtained by making the following substitutions in Eq. (8.15):

$$x^i \sim \zeta^{-1}m^{-1}, \quad \partial_i \sim \zeta m, \qquad \alpha^i \sim \zeta, \beta \sim 1, \quad R_{\alpha\beta\gamma\delta} \sim D^{-2}, \tag{9.1}$$

where D is a characteristic length or radius of curvature of the spacetime at the location of the atom. The quantity ζ defined in Eq. (8.11) is of the order $Z/137$, which we take to be small. The average electron velocity is of order ζ. In considering the nonrelativistic or low-velocity limit, we retain only the largest term in Eq. (8.15), obtaining

$$H_I \approx \tfrac{1}{2}mR_{0l0m}x^l x^m\beta, \tag{9.2}$$

which is of order $\zeta^{-2}m^{-1}D^{-2}$. Then

$$H \approx \vec{\alpha}\cdot\vec{p} + m\beta - \zeta r^{-1} + \tfrac{1}{2}mR_{0l0m}x^l x^m\beta, \tag{9.3}$$

where

$$p_i = -i\partial_i. \tag{9.4}$$

Using the standard representation

$$\alpha^i = \begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \tag{9.5}$$

and writing

$$\psi = \begin{pmatrix} \phi \\ \chi \end{pmatrix}, \tag{9.6}$$

one obtains from Eq. (8.1) the two-component equations

$$\vec{\sigma}\cdot\vec{p}\chi + (m - \zeta r^{-1} + \tfrac{1}{2}mR_{0l0m}x^l x^m)\phi = E\phi, \tag{9.7}$$

and

$$\vec{\sigma}\cdot\vec{p}\phi = (E + m + \zeta r^{-1} + \tfrac{1}{2}mR_{0l0m}x^l x^m)\chi. \tag{9.8}$$

For the gravitational $\frac{1}{2}mR_{0l0m}x^l x^m$ term not to disrupt the atom, it is necessary that the term not be as large as the electrostatic ζr^{-1} term, which implies that $\zeta^{-2}m^{-1}D^{-2} < \zeta^2 m$, or

$$D > \zeta^{-2}m^{-1} = Z^{-2}(7 \times 10^{-7}\ \text{cm}). \tag{9.9}$$

Solving Eq. (9.8) for χ and substituting into Eq. (9.7) gives

$$(E+m)^{-1}\vec{p}^2\phi - (E+m)^{-2}(\zeta r^{-1} + \tfrac{1}{2}mR_{0l0m}x^l x^m)\vec{p}^2\phi - (\zeta r^{-1} - \tfrac{1}{2}mR_{0l0m}x^l x^m)\phi = (E-m)\phi, \tag{9.10}$$

where we used $(\vec{\sigma}\cdot\vec{p})^2 = \vec{p}^2$ and expanded the denominator of the term involving $\vec{p}^2$. The first and third terms multiplying ϕ on the left side of Eq. (9.10) are each of order $\zeta^2 m$, while the second term is of order $\zeta^4 m$ and can be neglected in the nonrelativistic limit. It is then consistent to retain $\frac{1}{2}mR_{0l0m}x^l x^m$ in the third term on the left side of Eq. (9.10) only if one requires that $\zeta^{-2}m^{-1}D^{-2} > \zeta^4 m$, or

$$D < \zeta^{-3}m^{-1} = Z^{-3}(1 \times 10^{-4}\ \text{cm}). \tag{9.11}$$

If D exceeds the limit in Eq. (9.11), the gravitational effects will be too weak to include in the nonrelativistic limit of the Dirac equation. Thus, noting that $(E+m)^{-1}\vec{p}^2 = (2m)^{-1}\vec{p}^2 + O(\zeta^4 m)$, and neglecting terms of order $\zeta^4 m$, we obtain the nonrelativistic limit

$$H_{\rm NR}\phi = W\phi, \tag{9.12}$$

with

$$H_{\rm NR} = (2m)^{-1}\vec{p}^2 - \zeta r^{-1} + \tfrac{1}{2}mR_{0l0m}x^l x^m \tag{9.13}$$

and

$$W = E - m. \tag{9.14}$$

For the classical Hamiltonian corresponding to $H_{\rm NR}$, one has

$$dp_i/dt = -\partial H_{\rm NR}/\partial x^i = -\zeta x^i r^{-3} - mR_{0l0m}x^m. \tag{9.15}$$

The last term in Eq. (9.15) is the same as the well-known classical geodesic deviation force (Ref. 8, p.34), with m being the reduced mass.

In the nonrelativistic regime defined by Eq. (9.11), one expects the gravitational shifts in the proper energy levels to dominate over the fine structure produced by the relativistic effects of the electron's velocity and spin. In the nonrelativistic regime, one can readily carry out the perturbation theory based on the nonrelativistic hydrogenic wave functions with the curvature interaction term appearing in Eq. (9.13). One finds that the shift in the energy of the $1S$ level to first order is

$$E^{(1)}(1S) = \tfrac{1}{2}\zeta^{-2}m^{-1}R_{00}\,, \tag{9.16}$$

and that of the $2S$ level is

$$E^{(1)}(2S) = 7\zeta^{-2}m^{-1}R_{00}\,. \tag{9.17}$$

For the $2P$ states, the matrix elements appearing in Eq. (5.15) are

$$\tfrac{1}{2}mR_{0i0j}(\psi_{21m}, x^i x^j \psi_{21m'})_0 \equiv H_{mm'}\,. \tag{9.18}$$

As R_{0i0j} is symmetric in i,j, one can choose the orientation of the spatial axes of the normal coordinates such that R_{0i0j} is diagonal. With R_{0i0j} diagonal, the matrix elements of Eq. (9.18) are

$$\begin{aligned} H_{00} &= 3\zeta^{-2}m^{-1}(R_{00} + 2R_{0z0z})\,,\\ H_{11} &= 3\zeta^{-2}m^{-1}(2R_{00} - R_{0z0z})\,,\\ H_{1,-1} &= H_{-1,1} = 3\zeta^{-2}m^{-1}(R_{0y0y} - R_{0x0x})\,,\\ H_{01} &= H_{10} = H_{0,-1} = H_{-1,0} = 0\,, \end{aligned} \tag{9.19}$$

and the solutions of the cubic equation

$$\det[H_{mm'} - E^{(1)}\delta_{mm'}] = 0 \tag{9.20}$$

are

$$E_1^{(1)}(2P) = 3\zeta^{-2}m^{-1}(R_{00} + 2R_{0x0x})\,, \tag{9.21}$$

$$E_2^{(1)}(2P) = 3\zeta^{-2}m^{-1}(R_{00} + 2R_{0y0y})\,, \tag{9.22}$$

and

$$E_3(2P) = 3\zeta^{-2}m^{-1}(R_{00} + 2R_{0z0z})\,. \tag{9.23}$$

Note that the perturbations of the $2P$ levels do not vanish when $R_{\mu\nu}$ vanishes. We now return to the relativistic regime, in which $D > \zeta^{-3}m^{-1}$ and the effects of curvature are perturbations on the relativistic fine structure.

X. GRAVITATIONAL PERTURBATION OF THE RELATIVISTIC ONE-ELECTRON ATOM: THE $1S_{1/2}$ STATES

In the relativistic regime, the gravitational interaction of Eq. (8.15) acts as a perturbation of the relativistic fine structure. Therefore, the known exact solutions of the Dirac equation for the one-electron atom in flat spacetime serve as the basis for the perturbation theory. Other small perturbations, such as nuclear effects, radiative corrections, and the relativistic correction to the value of the reduced mass, would of course be added to the gravitational perturbation calculated here. In the present paper, we will deal with the $1S_{1/2}$, $2S_{1/2}$, and $2P_{1/2}$ levels. The $2P_{1/2}$ levels are the lowest lying of the $n=2$ energy levels (when the Lamb shift is taken into account). Electric dipole transitions from the $2P_{1/2}$ to the $1S_{1/2}$ and $2S_{1/2}$ levels are permitted. In this section, we carry out the calculation for the $1S_{1/2}$ states to all orders in ζ. In the next section, we calculate the perturbations of the $2S_{1/2}$ and $2P_{1/2}$ levels to leading order in ζ.

For the one-electron atom described by the unperturbed Hamiltonian H_0 of Eq. (8.14), one commonly uses a representation which diagonalizes the commuting observables H_0, $\vec{J}^2$, J_z, and K, where

$$\vec{J} = \vec{L} + \tfrac{1}{2}\vec{\sigma}' \tag{10.1}$$

is the sum of the orbital angular momentum $\vec{L}$ and the spin angular momentum $\frac{1}{2}\vec{\sigma}'$, where

$$\vec{\sigma}' = \begin{bmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{bmatrix}, \tag{10.2}$$

and $\vec{\sigma}$ consists of the 2×2 Pauli matrices in the standard representation. The operator K is given by

$$K = \beta(\vec{\sigma}'\cdot\vec{L} + 1)\,. \tag{10.3}$$

The eigenvalues k of the operator K are such that

$$|k| = (J + \tfrac{1}{2})\,, \tag{10.4}$$

where $J(J+1)$ is an eigenvalue of $\vec{J}^2$. The energy eigenvalues are

$$E_{nJ} = m\{1 + \zeta^2[n - |k| + (k^2 - \zeta^2)^{1/2}]^{-2}\}^{-1/2}\,, \tag{10.5}$$

where ζ was defined in Eq. (8.11) and $n = 1, 2, \ldots$ is the principal quantum number.

The eigenstates of H_0 are labeled by the quantum numbers n, J, M, and $\tilde{\omega}$, where M is the eigenvalue of J_z and

$$\tilde{\omega} = k/|k| \tag{10.6}$$

is the sign of the eigenvalue of K. The parity operator is

$$P = \beta P^{(0)}\,, \tag{10.7}$$

where $P^{(0)}$ is the usual "orbital" parity operator which takes $\vec{r}$ into $-\vec{r}$. The energy eigenfunctions $\psi^M_{n\tilde{\omega}J}$ can be shown to have parity eigenvalue

$$P' = (-1)^{J+\tilde{\omega}/2}\,. \tag{10.8}$$

The orbital angular momentum quantum number,

l, of the nonrelativistic state corresponding to $\psi^{M}_{n\tilde{\omega}J}$ (i.e., of the upper two, or "large", components of ψ in the standard representation) is given by

$$l = J + \tfrac{1}{2}\tilde{\omega}. \tag{10.9}$$

There are two $1S_{1/2}$ ($n=1$, $l=0$, $J=\frac{1}{2}$) states, corresponding to $M=\pm\frac{1}{2}$, for which $\tilde{\omega}=-1$ and $P'=1$ (even parity). Those states can be written in the standard representation as[10]

$$\psi_{+}=\frac{1}{r\sqrt{4\pi}}\begin{pmatrix} F(r) \\ 0 \\ -iG(r)\cos\theta \\ -iG(r)\sin\theta e^{i\phi}\end{pmatrix} \tag{10.10}$$

and

$$\psi_{-}=\frac{1}{r\sqrt{4\pi}}\begin{pmatrix} 0 \\ F(r) \\ -iG(r)\sin\theta e^{-i\phi} \\ iG(r)\cos\theta\end{pmatrix} \tag{10.11}$$

where ψ_+ corresponds to $M=\frac{1}{2}$ and ψ_- to $M=-\frac{1}{2}$, and

$$F(r)=m^{1/2}N(1+\gamma)^{1/2}(mr)^{\gamma}\exp(-\zeta mr), \tag{10.12}$$

$$G(r)=-m^{1/2}N(1-\gamma)^{1/2}(mr)^{\gamma}\exp(-\zeta mr), \tag{10.13}$$

with

$$\gamma=(1-\zeta^2)^{1/2}, \tag{10.14}$$

and

$$N=(2\zeta)^{\gamma+1/2}[2\Gamma(2\gamma+1)]^{-1/2}. \tag{10.15}$$

The unperturbed energy of the $1S_{1/2}$ states is $m\gamma$.

The gravitational perturbations are determined by Eq. (5.15) with the $\phi_a^{(0)}$ given by ψ_+ and ψ_-. Thus, we need the matrix elements

$$\langle H_I\rangle_{ab}\equiv(\psi_a, H_I\psi_b), \tag{10.16}$$

where the subscripts a, b take on the values plus or minus. Because both of the ψ_a are of even parity, only the terms in H_I [Eq. (8.15)] which are even with respect to the parity operator P [Eq. (10.7)] will contribute (x^l, ∂_l, α_l are odd, while r and β are even). The even terms in H_I are the first, second, fifth, ninth, tenth, and eleventh. After a lengthy calculation, we obtain the following results for those matrix elements:

$$-\frac{i}{2}R_{0l0m}\langle x^l x^m \alpha^i\partial_i\rangle_{ab}=-\delta_{ab}\tfrac{1}{12}(2\gamma+1)m^{-1}R_{00}, \tag{10.17}$$

$$-\frac{i}{6}R_{iljm}\langle x^l x^m \alpha^j\partial^i\rangle_{ab}=\delta_{ab}\tfrac{1}{72}(2\gamma+1)m^{-1}(R+2R_{00}), \tag{10.18}$$

$$\frac{i}{4}(R_{jm}-R_{0j0m})\langle\alpha^j x^m\rangle_{ab}=0, \tag{10.19}$$

$$-\tfrac{1}{12}\zeta(R_{lm}+3R_{0l0m})\langle x^l x^m\gamma^{-1}\rangle_{ab}=-\delta_{ab}\tfrac{1}{72}(2\gamma+1)m^{-1}(R+4R_{00}), \tag{10.20}$$

$$\tfrac{1}{12}\zeta(R+4R_{00})\langle r\rangle_{ab}=\delta_{ab}\tfrac{1}{24}(2\gamma+1)m^{-1}(R+4R_{00}), \tag{10.21}$$

$$\tfrac{1}{2}mR_{0l0m}\langle x^l x^m\beta\rangle_{ab}=\delta_{ab}\tfrac{1}{12}\zeta^{-2}\gamma(\gamma+1)(2\gamma+1)m^{-1}R_{00}. \tag{10.22}$$

Adding these results gives

$$\langle H_I\rangle_{ab}=\delta_{ab}\tfrac{1}{12}\zeta^{-2}\gamma(\gamma+1)(2\gamma+1)m^{-1}R_{00}+\delta_{ab}\tfrac{1}{72}(2\gamma+1)m^{-1}(3R+4R_{00}). \tag{10.23}$$

It follows that both of the $1S_{1/2}$ levels are shifted by the same perturbation:

$$E^{(1)}(1S_{1/2})=\tfrac{1}{12}\zeta^{-2}\gamma(\gamma+1)(2\gamma+1)m^{-1}R_{00}+\tfrac{1}{72}(2\gamma+1)m^{-1}(3R+4R_{00}). \tag{10.24}$$

This is in Fermi normal coordinates with R and R_{00} evaluated at the center of mass (or energy) of the atom. Equation (10.24) includes all terms linear in $R_{\alpha\beta\gamma\delta}$, and is good to all orders in ζ. The expression for $E^{(1)}(1S_{1/2})$ will be written in generally covariant form in Sec. XII below. Expanding $\gamma=(1-\zeta^2)^{1/2}$ in Eq. (10.24) gives

$$E^{(1)}(1S_{1/2})=\tfrac{1}{2}\zeta^{-2}m^{-1}R_{00}+\tfrac{1}{8}m^{-1}(R-3R_{00})+O(\zeta^2 m^{-1}D^{-2}). \tag{10.25}$$

The leading term in Eq. (10.25) agrees with the corresponding expression in Eq. (9.16) for the nonrelativistic regime.

XI. GRAVITATIONAL PERTURBATION OF THE RELATIVISTIC $2S_{1/2}$ AND $2P_{1/2}$ LEVELS

For $n=2$ and $J=\frac{1}{2}$, there are four eigenstates of H_0 of Eq. (8.14), corresponding to the energy eigenvalue

$$E_{2,1/2}=m[1+\zeta^2(1+\gamma)^{-2}]^{-1/2}. \tag{11.1}$$

Two of those states are the $2S_{1/2}$ states ($n=2$, $l=0$, $J=\frac{1}{2}$) and two are the $2P_{1/2}$ states ($n=2$, $l=1$, $J=\frac{1}{2}$). According to Eqs. (10.8) and (10.9), the $2S_{1/2}$ states have even parity and the $2P_{1/2}$ states have odd parity. Therefore, matrix elements of the leading term, $\frac{1}{2}\zeta mR_{0l0m}x^l x^m\beta$, in Eq. (8.15) will vanish between a $2S_{1/2}$ and a $2P_{1/2}$ state; to order $\zeta^{-2}m^{-1}D^{-2}$ there is no mixing of the $2S_{1/2}$ and $2P_{1/2}$ states. We calculate here the perturbation

of the $2S_{1/2}$ and $2P_{1/2}$ levels to leading order. In later work we intend to calculate these perturbations to higher order, including the mixing of the $2S_{1/2}$ and $2P_{1/2}$ levels, and to calculate the perturbations of the $2P_{3/2}$ levels.

The $2S_{1/2}$ states have the same form as the $1S_{1/2}$ states in Eqs. (10.10) and (10.11), except that for the $2S_{1/2}$ states $F(r)$ and $G(r)$ are[10]

$$F(r) = m^{1/2}N(1+W)^{1/2}(mr)^{\gamma} \times \exp[-\zeta mr(2W)^{-1}](c_0 + c_1 mr), \quad (11.2)$$

$$G(r) = -m^{1/2}N(1-W)^{1/2}(mr)^{\gamma} \times \exp[-\zeta mr(2W)^{-1}](2 + c_0 + c_1 mr), \quad (11.3)$$

with γ defined in Eq. (10.14), and

$$W = [(1+\gamma)/2]^{1/2}, \quad (11.4)$$

$$c_0 = 2W, \quad c_1 = -\zeta(2W+1)W^{-1}(2\gamma+1)^{-1}, \quad (11.5)$$

and

$$N = \tfrac{1}{2}(2\zeta)^{\gamma+1/2}(2W)^{-\gamma-1}\left(\frac{2\gamma+1}{(2W+1)\Gamma(2\gamma+1)}\right)^{1/2}. \quad (11.6)$$

The perturbations are determined by the matrix elements $\langle H_I\rangle_{ab}$ of the same form as in Eq. (10.16), but involving the $2S_{1/2}$ states, rather than the $1S_{1/2}$ states. As we are now working only to leading order in ζ, only the leading term in H_I need be retained:

$$H_I = \tfrac{1}{2}mR_{0l0m}x^l x^m\beta + \text{higher order in } \zeta. \quad (11.7)$$

One finds that for the $2S_{1/2}$ states,

$$\langle x^l x^m\beta\rangle_{ab} = \delta_{ab}\delta^{lm}14\zeta^{-2}m^{-2}. \quad (11.8)$$

Therefore

$$\langle H_I\rangle_{ab} = \delta_{ab}7\zeta^{-2}m^{-1}R_{00}, \quad (11.9)$$

and both $2S_{1/2}$ levels are shifted, to order $\zeta^{-2}m^{-1}D^{-2}$, by the same quantity:

$$E^{(1)}(2S_{1/2}) = 7\zeta^{-2}m^{-1}R_{00}, \quad (11.10)$$

which is the same as the nonrelativistic result in Eq. (9.17).

The $2P_{1/2}$ states in the standard representation are[10]

$$\psi_+ = \frac{1}{r\sqrt{4\pi}}\begin{pmatrix} -F(r)\cos\theta \\ -F(r)\sin\theta e^{i\phi} \\ iG(r) \\ 0 \end{pmatrix}, \quad (11.11)$$

and

$$\psi_- = \frac{1}{r\sqrt{4\pi}}\begin{pmatrix} -F(r)\sin\theta e^{-i\phi} \\ F(r)\cos\theta \\ 0 \\ iG(r) \end{pmatrix}, \quad (11.12)$$

where $\psi_\pm$ corresponds to $M = \pm\frac{1}{2}$, and

$$F(r) = m^{1/2}N(1+W)^{1/2}(mr)^{\gamma} \times \exp[-\zeta mr(2W)^{-1}](c_0 + c_1 mr), \quad (11.13)$$

$$G(r) = -m^{1/2}N(1-W)^{1/2}(mr)^{\gamma} \times \exp[-\zeta mr(2W)^{-1}](2W + c_1 mr), \quad (11.14)$$

with γ defined in Eq. (10.14), and

$$W = [(1+\gamma)/2]^{1/2}, \quad (11.15)$$

$$c_0 = 2(W-1), \quad (11.16)$$

$$c_1 = -\zeta(2W-1)W^{-1}(2\gamma+1)^{-1}, \quad (11.17)$$

and

$$N = \tfrac{1}{2}(2\zeta)^{\gamma+1/2}(2W)^{-\gamma-1}\left(\frac{2\gamma+1}{(2W-1)\Gamma(2\gamma+1)}\right)^{1/2}. \quad (11.18)$$

In order to apply Eq. (5.15) with the $\phi_a^{(0)}$ given by ψ_+ and ψ_- for the $2P_{1/2}$ states, we must calculate

$$\langle H_I\rangle_{ab} \equiv (\psi_a, H_I\psi_b), \quad (11.19)$$

where the subscripts a, b take on the values + or −, and to lowest order H_I is given by Eq. (11.7). To lowest order in ζ, one finds that

$$\langle x^l x^m\beta\rangle_{ab} = \delta_{ab}\delta^{lm}10\zeta^{-2}m^{-2}, \quad (11.20)$$

and hence,

$$\langle H\rangle_{ab} = \delta_{ab}5\zeta^{-2}m^{-1}R_{00}. \quad (11.21)$$

It follows that both $2P_{1/2}$ levels are shifted by the same quantity to order $\zeta^{-2}m^{-1}D^{-2}$, namely,

$$E^{(1)}(2P_{1/2}) = 5\zeta^{-2}m^{-1}R_{00}. \quad (11.22)$$

Calculation of the energy shifts of the $2P_{3/2}$ levels is underway. One expects those shifts to involve R_{0i0j} in a manner analogous to the shifts of the nonrelativistic $2P$ levels given in Eqs. (9.21)–(9.23).

XII. SUMMARY AND CONCLUSIONS

The energy shifts $E^{(1)}$ obtained above are those which would be measured by a detector located near the atom and at rest relative to it. A distant observer would see additional Doppler, gravitational, and cosmological shifts affecting all spectral lines uniformly, and thus separable from the

effects calculated here. The perturbations calculated here to first order in the Riemann tensor are all of the form

$$E^{(1)} = AR_{00} + BR + \sum_{i=1}^{3} C^{ii} R_{0i0i}\,, \tag{12.1}$$

Where R_{00} and R_{0i0j} are evaluated at the center of mass of the atom in a locally inertial proper frame with spatial axes oriented along the principal directions of R_{0i0j}. The constants A, B, and C^{ii} depend on the state, and for the cases studied are as follows (only the coefficients which do not vanish to the order considered are listed).

Nonrelativistic regime:

$$1S \text{ level: } A = \tfrac{1}{2}\zeta^{-2}m^{-1}\,, \tag{12.2}$$

$$2S \text{ level: } A = 7\zeta^{-2}m^{-1}\,, \tag{12.3}$$

$$2P \text{ levels: (1) } A = 3\zeta^{-2}m^{-1},\quad C^{11} = 6\zeta^{-2}m^{-1}\,, \tag{12.4}$$

$$\text{(2) } A = 3\zeta^{-2}m^{-1},\quad C^{22} = 6\zeta^{-2}m^{-1}\,, \tag{12.5}$$

$$\text{(3) } A = 3\zeta^{-2}m^{-1},\quad C^{33} = 6\zeta^{-2}m^{-1}\,. \tag{12.6}$$

Relativistic regime:

$$1S_{1/2} \text{ levels: } A = \tfrac{1}{12}\zeta^{-2}\gamma(\gamma+1)(2\gamma+1)m^{-1} + \tfrac{1}{18}(2\gamma+1)\,,$$
$$B = \tfrac{1}{24}(2\gamma+1)m^{-1} \tag{12.7}$$

$$2S_{1/2} \text{ levels: } A = 7\zeta^{-2}m^{-1}\,, \tag{12.8}$$

$$2P_{1/2} \text{ levels: } A = 5\zeta^{-2}m^{-1}\,, \tag{12.9}$$

where

$$\zeta = Ze^2,\quad \gamma = (1-\zeta^2)^{1/2}\,. \tag{12.10}$$

Here Eq. (12.7) is exact, while the other results are valid to order $\zeta^{-2}m^{-1}$. For the relativistic $2P_{3/2}$ levels, as for the nonrelativistic $2P$ levels, the constants C^{ii} will not vanish.

Given a set of sufficiently narrow spectral lines, and expressions like Eq. (12.1) for the perturbations $E^{(1)}$ of the energy levels involved in the observed transitions, one could hope to measure or put upper bounds on components of the Riemann tensor in the proper frame of the atom. Such an analysis would give objective information about the curvature at the position of the atom, independent of the mechanism producing that curvature.

Conversely, given a spacetime metric, one can calculate the components of the Riemann tensor in Eq. (12.1) in order to predict the spectral frequency shifts. The components of the Riemann tensor appearing in Eq. (12.1) are evaluated at the origin of a locally inertial rest frame of the atom (referred to below as "the proper frame"). In the following equations, indices with a caret refer to the proper frame, while other indices refer to arbitrary coordinates. The components in the proper frame with spatial axes oriented along the principal directions of $R_{\hat{0}\hat{i}\hat{0}\hat{j}}$ are related to the components in arbitrary coordinates by the following equations:

$$R_{\hat{0}\hat{0}} = R_{\mu\nu}u^{\mu}u^{\nu}\,, \tag{12.11}$$

where

$$u^{\mu} = dx^{\mu}/d\tau \tag{12.12}$$

is the four-velocity of the atom, having components $u^{\hat{\mu}} = \delta^{\mu 0}$ in the proper frame. Also,

$$R_{\hat{0}\hat{i}\hat{0}\hat{j}} = R_{\mu\nu\lambda\sigma}u^{\mu}\zeta_i^{\nu}u^{\lambda}\zeta_j^{\sigma}\,, \tag{12.13}$$

where the three spacelike unit vectors ζ_i^{μ} $(i=1,2,3)$ are chosen (i) to be orthogonal to u^{μ} and (ii) so that $R_{\mu\nu\lambda\sigma}u^{\mu}\zeta_i^{\nu}u^{\lambda}\zeta_j^{\sigma}$ is diagonal in the indices i and j (the diagonalization can be accomplished in general because of the symmetry under interchange of i and j).

It follows from Eqs. (12.11)–(12.13) that motion of the atom relative to a curved spacetime will affect the rest energy of the atom. For example, in the static Einstein universe, if the atom is at rest relative to the globally static coordinate system then $R_{\hat{0}\hat{0}}$ vanishes and $E^{(1)}(1S_{1/2})$ is of order $m^{-1}R$, but if the atom is moving relative to the static coordinate system then $E^{(1)}(1S_{1/2})$ includes a nonvanishing term of order $\zeta^{-2}m^{-1}R_{\hat{0}\hat{0}}$. These effects do not violate the principle of equivalence because they are measurable only if the gravitational field changes significantly over the dimensions of the atom.

The results for the perturbations $E^{(1)}$ calculated above are contained in the covariant expression

$$P^{\lambda} = E^{(0)}u^{\lambda} + (AR_{\mu\nu}u^{\mu}u^{\nu} + BR + C^{ij}R_{\mu\nu\epsilon\sigma}u^{\mu}\zeta_i^{\nu}u^{\epsilon}\zeta_j^{\sigma})u^{\lambda}\,, \tag{12.14}$$

where P^{λ} is the energy-momentum four-vector of the atom, and $E^{(0)}$ is the rest energy of the atom in flat spacetime. The constants A, B, and C^{ij} are the same as in Eqs. (12.2)–(12.9), with the ones not explicitly listed taken to be zero to the order under consideration. The three spacelike unit vectors ζ_i^{μ}, which are orthogonal to u^{μ} and point along the principal axes of R_{0i0j} in normal coordinates, are the same vectors as in Eq. (12.13). The above equation for P^{λ} is the covariant expression which reduces to $P^{i}=0$, $P^{0} = E^{(0)} + E^{(1)}$ in the proper frame of the atom.

The energy-level shifts caused by the local curvature of spacetime will be of the same order of magnitude as the Lamb shift in hydrogen when the following condition is satisfied:

$$\zeta^{-2}m^{-1}D^{-2} \approx 4\times 10^{-6}\ \text{eV}\,.$$

The characteristic radius of curvature leading to

energy shifts of that magnitude is thus

$$D \approx 2 \times 10^{-3} \text{ cm}. \tag{12.15}$$

Within the context of the theory of general relativity, one would expect regions of such large curvature to exist in the vicinity of small black holes left over from the early stages of the universe. For the Schwarzschild metric with the atom at the Schwarzschild radial coordinate r_S and moving along the radial direction, one can diagonalize $R_{\hat{0}\hat{i}\hat{0}\hat{j}}$ by choosing the $\hat{x}$-axis of the normal coordinates in the radial direction. Then one has[7] $R_{\hat{0}\hat{x}\hat{0}\hat{x}} = -2Mr_S^{-3}$, $R_{\hat{0}\hat{y}\hat{0}\hat{y}} = R_{\hat{0}\hat{z}\hat{0}\hat{z}} = +Mr_S^{-3}$, where M is the Schwarzschild mass (in the present units, $G = c = \hbar = 1$), and the velocity of the atom does not appear in this highly symmetrical example. In this case, the $2P$ level is split into two levels with [see Eqs. (9.21)–(9.23)]

$$E_1^{(1)}(2P) = -12\zeta^{-2}m^{-1}Mr_S^{-3}, \tag{12.16}$$

and

$$E_2^{(1)}(2P) = E_3^{(1)}(2P) = +6\zeta^{-2}m^{-1}Mr_S^{-3}. \tag{12.17}$$

The shifts of the relativistic $2P_{3/2}$ levels are expected to also be proportional to $\zeta^{-2}m^{-1}Mr_S^{-3}$. Thus, if one could observe the spectrum of a hydrogen atom falling radially into a black hole having Schwarzschild radius of, say, 10^{-4} cm, then the above shifts would be of the order of 10^{-3} eV, which is much larger (by a factor of 100) than the relativistic fine structure. One can readily conceive of other idealized situations in which the effect of the curvature on the atom is observable. It would be desirable to construct plausible astrophysical models for which this effect is observable from far away.

From an experimental viewpoint, observations of atomic spectra can be used as a probe in searching for regions of significant curvature which may exist on a smaller scale than has previously been studied. Knowing the detailed dependence of the energy level shifts on the curvature tensor would permit the effects of curvature to be distinguished from other possible perturbations of the energy levels. The framework set up in these papers can serve as a starting point for calculating the perturbations of more energy levels, and for extending the work to higher order in the Riemann curvature tensor. One may hope that, in addition to their intrinsic theoretical interest, these results may eventually permit one to use spectra to measure or put upper limits on the local curvature of distant regions of spacetime.

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