One-Electron Atom in Curved Space-Time

Leonard Parker
Department of Physics, University of Wisconsin–Milwaukee, Milwaukee, Wisconsin 53201
(Received 7 March 1980)

A one-electron atom in a general curved space-time is considered. The Hamiltonian of the Dirac equation is found in Fermi normal coordinates, and expressions are obtained, to first order in the Riemann tensor, for the shifts in energy of the $1S_{1/2}$, $2S_{1/2}$, and $2P_{1/2}$ levels.

PACS numbers: 98.80.Dr, 04.90.+e, 31.10.+z

The energy levels of an atom placed in a region of curved space-time will be shifted as a result of the interaction of the atom with the local curvature. This effect differs from the usual gravitational and Doppler shifts in that it perturbs each energy level to a different extent. Thus, in principle, atomic spectra carry unambiguous information about the local curvature at the position of the atom. These shifts would be appreciable only in regions of large curvature. For example, my results show that for the energy level shifts in hydrogen to be of the order of the Lamb shift (4.4×10^{-6} eV), the characteristic radius of curvature of space-time would have to be about 10^{-3} cm. Nevertheless, any effect which can allow one to unambiguously place upper limits on (or possibly measure) the local curvature of distant regions is of interest.

The calculation of the energy levels of a one-electron atom is curved space-time also presents interesting problems of a theoretical nature. There are contradictory conclusions in the literature, and to our knowledge no one has given explicit expressions for the energy level shifts, as I do here. A critique of the previous literature, including references, is given by Audretsch and Schäfer,[1] who considered the hydrogen atom in certain cosmological metrics.

I assume (i) that a metric description of space-time is valid, (ii) that the generally covariant Dirac equation governs the system, (iii) that, to good approximation, the atom is in free fall along a geodesic of the space-time during the time required for an atomic transition, and (iv) that the time rate of change of the Riemann tensor as measured along the space-time path of the atom is sufficiently small on an atomic time scale that well-defined energy levels exist. The metric is otherwise arbitrary.[2]

The Dirac equation is[3,4]

$$[\gamma^{\mu}(x)\nabla_{\mu}+m]\psi(x)=0, \tag{1}$$

where

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

and ∇_{μ} denotes the covariant derivative acting on the four-component spinor field $\psi(x)$. Minimal coupling to the electromagentic field is included in our definition of ∇_{μ}. One can show that the conserved scalar product, which reduces to the usual scalar product in flat space-time, and which has the properties required of a scalar product in a Hilbert space, is

$$(\varphi,\psi)\equiv -i\int d^3x\sqrt{-g}\,\varphi^{\dagger}\beta\gamma^0(x)\psi, \tag{3}$$

where β is the standard Dirac β matrix (the proof is based on the probability current density introduced in Ref. 4). The Hamiltonian form of Eq. (1) is

$$i\partial_0\psi=H\psi \tag{4}$$

with

$$H=-i(g^{00})^{-1}\gamma^0\gamma^i(\partial_i-\Gamma_i)+i\Gamma_0-i(g^{00})^{-1}\gamma^0 m, \tag{5}$$

where the Γ_{μ} are the spinor affine connections, including an additional term $-ieA_{\mu}1$, where e is the magnitude of the electron charge and A_{μ} is the electromagnetic vector potential. If time derivatives of the Riemann tensor in a locally inertial proper frame of the atom are neglected in accordance with assumption (iv) above, one finds that H is Hermitian with respect to the scalar product of Eq. (3). I may therfore interpret H as the observable corresponding to the energy of the system.

In Fermi normal coordinates,[5] each spacelike hypersurface of constant x^0 is generated by the set of spacelike geodesics normal at a point to the timelike geodesic G along which the atom is falling. The time x^0 of an event in the hypersurface is the proper time along G at the point where it intersects the hypersurface. These coordinates are normal along the geodesic G. Therefore, Fermi normal coordinates are appropriate for a problem involving energy levels (in contrast, for

example, to Riemann normal coordinates which are only normal in a neighborhood of a space-time point). The metric in these coordinates takes the form to first order in the Riemann tensor[6,7]:

$$g_{00}=-1-R_{0l0m}x^l x^m,\quad g_{0i}=-\tfrac{2}{3}R_{0lim}x^l x^m,\quad g_{ij}=\delta_{ij}-\tfrac{1}{3}R_{iljm}x^l x^m, \tag{6}$$

where Latin indices range from 1 to 3, and $R_{\mu\nu\lambda\sigma}$ is evaluated at the point at which the constant x^0 hypersurface intersects G [$R_{\mu\nu\lambda\sigma}$ is regarded as a slowly varying function of x^0 in accordance with assumption (iv)]. The curvature appearing here is that of the background geometry which I seek to measure, and not that generated by the atom itself.

I find to first order in the curvature that the electromagnetic vector potential produced by a point of charge Ze is

$$A_0=-Zer^{-1}+\tfrac{1}{12}Ze(R+4R_{00})r+\tfrac{1}{12}Ze(3R_{l0m}{}^0-R_{lm})x^l x^m r^{-1}, \tag{7}$$

and

$$A_k=\tfrac{1}{2}ZeR_{0k}r+\tfrac{1}{6}ZeR_{lkm}{}^0x^l x^m r^{-1}. \tag{8}$$

(Effects of finite nuclear size would be treated as an additive perturbation.) After a long calculation, one finds that the Hamiltonian of Eq. (5) is

$$H=H_0+H_I, \tag{9}$$

with

$$H_0=-i\alpha^i\partial_i+m\beta-\zeta r^{-1}, \tag{10}$$

and

$$\begin{aligned}H_I=&-\frac{i}{2}R_{0l0m}x^l x^m\alpha^i\partial_i-\frac{i}{6}R_{iljm}x^l x^m\alpha^j\partial^i-\frac{i}{6}R_{0ljm}x^l x^m\alpha^j\alpha^i\partial_i-\frac{i}{2}R_{0lim}x^l x^m\partial^i\\&+\frac{i}{4}\alpha^j(R_{jm}-R_{0j0m})x^m+\frac{i}{4}\alpha^i\alpha^jR_{0imj}x^m+\tfrac{1}{6}\zeta R_{0lmi}x^l x^m\alpha^i r^{-1}+\tfrac{1}{2}\zeta R_{0i}\alpha^i r\\&-\tfrac{1}{12}\zeta(R_{lm}+3R_{0l0m})x^l x^m r^{-1}+\tfrac{1}{12}\zeta(R+4R_{00})r+\tfrac{1}{2}mR_{0l0m}x^l x^m\beta-\tfrac{1}{6}mR_{il0m}x^l x^m\beta\alpha^i,\end{aligned} \tag{11}$$

where $\zeta=Ze^2$, and the α^i and β are the standard Dirac matrices. This result includes all terms of first order in the curvature tensor. I have checked by direct calculation that H of Eq. (9) is Hermitian with respect to the scalar product of Eq. (3). On the other hand, neither H_0 nor H_I alone is Hermitian with respect to that scalar product.

Therefore, one must exercise care in developing the perturbation theory of stationary states based on the flat space-time relativistic Hamiltonian H_0. Working to first order in the curvature, I find after calculation that the energy level shifts $E_i^{(1)}$ $(i=1,\ldots,n)$ of an n-fold degenerate energy level $E^{(0)}$ are determined by the equation

$$\det[(\psi_a^{(0)},H_I\psi_b^{(0)})_0-E_i^{(1)}\delta_{ab}]=0, \tag{12}$$

where the $\psi_a^{(0)}$ $(a=1,\ldots,n)$ are n orthonormal eigenvectors of H_0 corresponding to the degenerate eigenvalue $E^{(0)}$, and the subscript "0" on the scalar product denotes the usual flat-space-time scalar product

$$(\varphi,\psi)_0=\int d^3x\,\varphi^\dagger\psi. \tag{13}$$

[For convenience, we will refer to Eq. (13) as the flat scalar product and Eq. (3) as the curved scalar product. The $\psi_a^{(0)}$ are orthonormal with respect to the flat scalar product.] The expression in Eq. (12) has the same appearance as in flat space-time, except that H_I is not Hermitian with respect to the flat (or curved) scalar product. The reality of the $E_i^{(1)}$ is assured by the Hermiticity of H with respect to the curved scalar product.

The orders of magnitude of the matrix elements of the various terms in H_I are obtained by making

the following substitutions in Eq. (11):

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

where D is the characteristic length or radius of curvature of the space-time at the location of the atom. The largest term in H_I is $\frac{1}{2} m R_{0l0m} x^l x^m \beta$, which is of order $\zeta^{-2} m^{-1} D^{-2}$, and corresponds in the nonrelativistic (low electron velocity) limit to the geodesic deviation term in the classical Hamiltonian (e.g., see p. 34 of Ref. 7 on the geodesic deviation force).

Inserting the known exact spinor solutions[8] of the eigenvalue problem for H_0 in the matrix elements of Eq. (12), I find after a lengthy calculation that both of the degenerate $1S_{1/2}$ levels are shifted by the same amount:

$$E^{(1)}(1S_{1/2}) = \tfrac{1}{12}\zeta^{-2}\gamma(\gamma+1)(2\gamma+1)m^{-1}R_{00} + \tfrac{1}{72}(2\gamma+1)m^{-1}(3R + 4R_{00}), \tag{14}$$

where

$$\gamma = (1-\zeta^2)^{1/2}, \quad \zeta = Ze^2. \tag{15}$$

This expression includes all terms linear in $R_{\alpha\beta\gamma\delta}$ and is valid to all orders in ζ. One expects a result to this order in the curvature to involve only R_{00} and R because $E^{(1)}$ must be invariant under the rotation of the spatial axes of a locally inertial rest frame of the atom. The quantities R and R_{00} are evaluated at the center of mass of the atom in a locally inertial rest frame of the atom, and m is the reduced mass. 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 curvature shift calculated here. Expanding γ in Eq. (14) gives

$$E^{(1)}(1S_{1/2}) = \tfrac{1}{2}\zeta^{-2}m^{-1}R_{00} + \tfrac{1}{8}m^{-1}(R - 3R_{00}) + O(\zeta^2 m^{-1} D^{-2}). \tag{16}$$

The degeneracy of the $1S_{1/2}$ levels is not removed to first order in the curvature. I intend to carry the calculation to second order in the curvature, which should result in a splitting of the $1S_{1/2}$ levels.

The $2S_{1/2}$ and $2P_{1/2}$ eigenstates of H_0 are fourfold degenerate. One can use parity selection rules to show that the matrix elements of the largest term in H_I, namely $\frac{1}{2} m R_{0l0m} x^l x^m \beta$, vanish when taken between a $2S_{1/2}$ state and a $2P_{1/2}$ state. Therefore, to lowest order in ζ the $2S_{1/2}$ and $2P_{1/2}$ levels are not mixed. I find that, in lowest order, the energy of the $2S_{1/2}$ states is separated from that of the $2P_{1/2}$ states, and each of the resulting energy levels is twofold degenerate. The energy shifts are, to lowest order in ζ,

$$E^{(1)}(2S_{1/2}) = 7\zeta^{-2}m^{-1}R_{00}, \tag{17}$$

and

$$E^{(1)}(2P_{1/2}) = 5\zeta^{-2}m^{-1}R_{00}. \tag{18}$$

The terms of lowest order in ζ in Eq. (16) and Eq. (17) are the same as would be obtained by use of the geodesic deviation interaction, $\frac{1}{2} m R_{0l0m} x^l x^m$, with the nonrelativistic Schrödinger equation. However, the results given above also hold when the curvature term is too small to be retained in the nonrelativistic limit of the Dirac equation. The splitting of the $2S_{1/2}$ and $2P_{1/2}$ levels in hydrogen caused by the curvature will be of the same order as that caused by the Lamb shift (4.4×10^{-6} eV) when the characteristic radius of curvature, D, is about 10^{-3} cm. The nonrelativistic limit with the curvature term is valid in hydrogen for $D < 10^{-4}$ cm, when the perturbation would be larger than the relativistic fine structure, and would be readily observable.

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 the atom. 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 terms in $E^{(1)}$ calculated above vanish in a region where $R_{\mu\nu}$ is zero. However, that is not true for other energy levels or to higher order. For example, in the nonrelativistic regime, I find that the shifts in the three $2P$ levels are

$$E_1^{(1)} = 3\zeta^{-2}m^{-1}(R_{00} + 2R_{0x0x}), \quad E_2^{(1)} = 3\zeta^{-2}m^{-1}(R_{00} + 2R_{0y0y}), \quad E_3^{(1)} = 3\zeta^{-2}m^{-1}(R_{00} + 2R_{0z0z}), \tag{19}$$

where the x, y, and z directions of the normal coordinates have been chosen such that R_{0i0j} is diagonal at the origin. For the Schwarzschild metric with the x axis of the normal coordinates in the radial direction, one has[6] $R_{00}=0$, $R_{0x0x}=2Mr^{-3}$, and $R_{0y0y}=R_{0z0z}=-Mr^{-3}$, where M is the Schwarzschild mass ($G=1$) and r is the Schwarzschild radial coordinate. In future work, I will extend the present results in both the nonrelativistic and relativistic regimes. These results are independent of the theory by by which the curvature tensor $R_{\mu\nu\lambda\sigma}$ of the space-time is generated.

Finally, I note that the above expressions can be written covariantly with the aid of u^μ, the four-velocity of the atom, and the three spacelike unit vectors $\zeta_i{}^\mu (i=1,2,3)$ which are orthogonal to u^μ and point along the principal axes of R_{0i0j} in normal coordinates. The results for $E^{(1)}$ calculated above are contained in the covariant expression

$$P^\lambda = E^{(0)}u^\lambda + (AR_{\mu\nu}u^\mu u^\nu + BR + C^{ij}R_{\mu\nu\epsilon\sigma}u^\mu \zeta_i{}^\nu u^\epsilon \zeta_{j\sigma})u^\lambda, \tag{20}$$

where P^λ is the energy-momentum four-vector of the atom, $E^{(0)}$ is the rest energy of the atom in flat space-time, and the constants A, B, and C^{ij} are determined for the $1S_{1/2}$ level by Eq. (16), for the $2S_{1/2}$ and $2P_{1/2}$ levels to order $\zeta^{-2}m^{-1}D^{-2}$ by Eqs. (17) and (18), and for the $2P$ levels in the nonrelativistic regime by Eq. (19). It follows that the total rest energy of the atom is affected by its motion relative to a curved space-time.

The author thanks the National Science Foundation for support of this research under Grant No. PHY79-06657.

[1]J. Audretsch and G. Schäfer, Gen. Relativ. Gravitation 9, 243, 489 (1978).

[2]I do not consider nontrivial topologies.

[3]E. Schrödinger, Sitzungsber. Dtsch. Akad. Wiss. Berlin, Math. Naturwiss. Kl. 1932, 105 (1932).

[4]V. Bargmann, Sitzungsber. Dtsch. Akad. Wiss. Berlin, Math. Naturwiss. Kl. 1932, 346 (1932).

[5]E. Fermi, Atti R. Acad. Naz. Lincei Mem. Cl. Sci. Fis. Mat. Nat. 31, 21, 51 (1922).

[6]F. K. Manasse and C. W. Misner, J. Math. Phys. 4, 735 (1963).

[7]C. W. Misner, K. S. Thorne, and J. A. Wheeler, *Gravitation* (Freeman, San Francisco, 1973). I use the sign conventions of this reference.

[8]M. E. Rose, *Relativistic Electron Theory* (Wiley, New York, 1961).