The Energy-Level Shifts of a Stationary Hydrogen Atom in Static External Gravitational Field with Schwarzschild Geometry

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Abstract

The first order perturbations of the energy levels of a stationary hydrogen atom in static external gravitational field, with Schwarzschild metric, are investigated. The energy shifts are calculated for the relativistic 1S, 2S, 2P, 3S, 3P, 3D, 4S, 4P, 4D and 4F levels. The results show that the energy-level shifts of the states with total angular momentum quantum number 1/2 are all zero, and the ratio of absolute energy shifts with total angular momentum quantum number 5/2 is 1 : 4 : 5. This feature can be used to help us to distinguish the gravitational effect from other effect.

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I. INTRODUCTION

The study of gravitational fields interacting with spinor fields constitutes an important element in constructing a theory that combines quantum physics and gravity. For this reason, the investigation of the behavior of relativistic particles in this context is of considerable interest. With this interaction the energy levels of an atom placed in external gravitational field will be shifted. And these shifts, which would depend on the features of the spacetime, are different for each energy level. So they can be distinguished from the Doppler effect and from the gravitational and cosmological red-shifts, in which cases the shifts would be the same for all spectral lines. Thus the atomic spectra carries the information about the local curvature at the position of the atom. That may be led to a test of general relativity at the quantum level, and one can, in principle, use the atom as an instrument to detect possible regions of high curvature.

The hydrogen atom as the most simplest structure atom is an ideal object to study this interaction and to detect the space-time curvature. Using the Fermi normal coordinates the energy-level shifts of hydrogen in a region of curved space-time has been investigated in Refs. [1, 2, 3]. The Fermi normal coordinates require that the hydrogen atom is free falling along a geodesic. The mixing of opposite-parity states of an atom supported in gravitational field by non-gravitational forces was investigated in Ref. [4]. And that paper showed that the separation of center-of-mass and relative coordinates is a complicated problem and the form of Hamiltonian depends on the choice of center-of-mass and relative coordinates. We think our calculation is not relevant to the problem. Because, firstly, just like as the discussion in the last paragraph of the page 2164 in Ref. [4], that the mass of electron is much lighter than that of proton, so the problem can be neglected with good approximate. Secondly, with the same approach by Manasse and Misner in Ref. [7], we think that the separation of center-of-mass and relative coordinates has been solved comfortably. Because with the method of Manasse and Misner, the metric, connection, tetrad, etc., can be expanded with the Riemann tensor at relative coordinates, and the Riemann tensor is decided by the center-of-mass coordinate. So we think that we can neglect that problem in our paper.

In this paper we also investigate the energy-level shifts of a stationary hydrogen atom, with good approximately, in static external gravitational field with Schwarzschild metric. In
particular, we use Riemann normal coordinates which are only normal in a neighborhood of a space-time point. In this paper we prove the equivalence of the gravitation effects of a hydrogen atom freely falling along a radial geodesic [3] and resting in static external gravitational field. We also redo the calculation in this paper because in Ref. [3] the authors don’t calculate the parts of total angular momentum quantum number 5/2. And from our calculation, we find that the ratio of absolute energy shifts of those parts is 1:4:5, and the states with total angular momentum quantum number \( \frac{1}{2} \) are zero. We think these are good results and can be used to help us to separate the shifts in the energy levels caused by other effects.

In our earlier paper [12] we have investigated the first order perturbations of the energy levels of a hydrogen atom in central internal gravitational field, which is produced by the mass of the atomic nucleus. And the energy-level shifts are caused by interaction of electronic with internal gravitational field. In this paper we continue to study the energy-level shifts of a stationary hydrogen atom, which are caused by the static external gravitational field, with Schwarzschild metric. In this case we need to solve the problem of the separation of center-of-mass and relative coordinates, and which doesn’t appear in our earlier paper [12]. And the energy-level shifts are not fixed in this case with the uncertain of the mass of gravitation source and the position of the atom.

In this paper we use the space-time signature \((-,-,+,+,+))\). And under the transformations of coordinates Greek indices \(\mu, \nu, \ldots\), which imply values from 0 to 3, are regarded as the tensor indices lowered with the curved space-time metric \(g_{\mu\nu}\). While indices \(a,b,c,d\) (0 to 3) are the Lorentz group indices ‘lowering’ with flat space-time metric \(\eta_{ab}\).

This paper is organized as follows. In Sec. \(\text{III}\) we review the formalism of the Dirac equation in curved space-time. In Sec. \(\text{IV}\) metric and affinity are calculated in Riemann normal coordinates. In Sec. \(\text{V}\) we give the Riemann tensor in Riemann normal coordinates with Schwarzschild geometry. The relativistic energy shifts of the atom are calculated in Sec. \(\text{V}\). Finally, Sec. \(\text{VI}\) is the conclusion.
II. GENERALLY COVARIANT DIRAC EQUATION IN CURVED SPACE-TIME

The generally covariant form of the Dirac equation in gravitational and electromagnetic fields can be written as \[4, 6\]

\[ \Gamma_{\mu}(\partial_{\mu} - \omega_{\mu} - iqA_{\mu})\psi(x) + \frac{mc}{\hbar}\psi(x) = 0, \]  

(1)

where \( \Gamma_{\mu} \) is the generalized Dirac-Pauli matrices

\[ \Gamma_{\mu}(x) = b_{\mu}^{a}(x)\gamma_{a}, \]  

(2)

\( \omega_{\mu} \) is the spinor connection defined as

\[ \omega_{\mu} = \frac{1}{2}I_{\alpha\beta}(\nabla_{\mu}b_{\nu}^{\alpha})b_{\lambda}^{\beta}g^{\lambda\nu}, \]  

(3)

\( A_{\mu} \) is the electromagnetic vector potential in curved space-time, \( q = -e \) is the charge of electron, \( b_{\mu}^{a} \) is the tetrad (vierbein) field satisfying the relations

\[ g_{\mu\nu}(x) = \eta_{ab}b_{\mu}^{a}(x)b_{\nu}^{b}(x), \]  

(4)

\[ b_{\mu}^{a}(x)b_{\mu}^{a}(x) = \delta_{b}^{b}. \]  

(5)

And \( I_{ab} \) is the generator of \( SO(3,1) \) group, whose spinor representation is

\[ I_{ab} = \frac{1}{4}(\gamma_{a}\gamma_{b} - \gamma_{b}\gamma_{a}). \]  

(6)

Here \( \gamma_{a} \) are the Dirac-Pauli matrices with the following relation

\[ \gamma_{a}\gamma_{b} + \gamma_{b}\gamma_{a} = 2\eta_{ab}, \]  

(7)

and

\[ \gamma_{0} = -\gamma_{0}, \quad \gamma_{i} = \gamma_{i} \quad (i = 1, 2, 3), \]  

(8)

\[ \gamma_{0} = i\beta, \quad \gamma_{i} = -i\beta\alpha_{i}. \]  

(9)

\[ \alpha_{i} = \begin{pmatrix} 0 & \sigma_{i} \\ \sigma_{i} & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \]  

(10)

where \( I \) is the \( 2 \times 2 \) identity matrix, and \( \sigma_{i} \) are the standard Pauli matrices

\[ \sigma_{1} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_{2} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_{3} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \]  

(11)
III. METRIC AND AFFINITY IN RIEMANN NORMAL COORDINATES

To calculate the energy-level shifts for a stationary hydrogen in gravitational field, the Riemann normal coordinates is an ideal mathematic tool. The well known Riemann normal coordinates satisfy the conditions $g_{\mu\nu}|_{p_0} = \eta_{\mu\nu}|_{p_0}$ and $\Gamma^\mu_{\nu\lambda}|_{p_0} = 0$ at a point $p_0$—the origin of the coordinate system. For arbitrary point $p$ in some neighborhood $V(p_0)$ there is the unique geodic $\gamma(u)$ connecting $p_0$ and $p$, with $u$ being the canonical parameter. The Riemann normal coordinates defined as $x^\mu = u\xi^\mu$, where $\xi^\mu = dx^\mu/du$, with the origin at the point $p_0$. And a set of orthonormal vectors $\vec{e}_0, \vec{e}_1, \vec{e}_2, \vec{e}_3$ at the point $p_0$ fix the coordinate axes there. We assume that the hydrogen atom is stationary with good approximation at the space-time point $p_0$. So the Riemann normal coordinates are also stationary reference coordinates. Because the gravitational field we considered is static so the derivative with time is zero for all tensors and connections in Riemann normal coordinates. The first order derivatives of affine connection at the point $p_0$ are:

$$
\begin{align*}
\Gamma^\mu_{\nu\lambda,0} &= 0, \\
\Gamma^\mu_{0\nu,l} &= R^\mu_{\nu\lambda} l, \\
\Gamma^\mu_{ij,l} &= \frac{1}{3}(R^\mu_{ij} + R^\mu_{ji}),
\end{align*}
$$

(12)

where $\Gamma^\mu_{\nu\lambda,0} = \Gamma^\mu_{\nu\lambda,p}(p_0)$. Above formulas can be also got in Fermi normal coordinates, for the equation $\Gamma^\mu_{\nu\lambda}|_G = 0$ holds for all $x^0 = \tau$ at the timelike geodesic $G(\tau)$ in that frame. With the relation of

$$
\begin{align*}
g^\mu_{\nu,ab} = \eta_{\mu\nu} & \Gamma^\sigma_{\nu a,b} + \eta_{\sigma\nu} \Gamma^\mu_{\nu a,b},
\end{align*}
$$

(13)

the metric up to second order in these coordinates takes the form

$$
\begin{align*}
g_{00} &= -1 + \frac{1}{3} R_{0lm} x^l x^m, \\
g_{0j} &= g^{0j} = \frac{2}{3} R_{0jm} x^l x^m, \\
g_{ij} &= \delta_{ij} + \frac{1}{3} R_{ijm} x^l x^m, \\
g^{00} &= -1 - \frac{1}{3} R^0_{l m} x^l x^m, \\
g^{ij} &= \delta^{ij} - \frac{1}{3} R^i_{l m} x^l x^m.
\end{align*}
$$

(14)
Using the equation of parallel propagation in the Riemann normal coordinates

\[ \frac{db^\mu}{du} - \Gamma^\lambda_{\mu\sigma} b^\sigma \xi^\lambda = 0, \]

we can write the tetrad as

\begin{align*}
  b^a_0 &= \delta_0^a + \frac{1}{2} \Gamma^a_{0l,m} x^l x^m = \delta_0^a + \frac{1}{2} R^a_{0l} x^l x^m, \\
  b^a_\mu &= \delta_0^a - \frac{1}{2} \Gamma^a_{\mu l,m} x^l x^m = \delta_0^a - \frac{1}{2} R^a_{\mu l} x^l x^m, \\
  b^a_i &= \delta_i^a + \frac{1}{2} \Gamma^a_{i l,m} x^l x^m = \delta_i^a + \frac{1}{6} (R^a_{iml} + R^a_{mil}) x^l x^m = \delta_i^a + \frac{1}{6} R^a_{mil} x^l x^m, \\
  b^a_\mu &= \delta_i^a - \frac{1}{2} \Gamma^a_{i l,m} x^l x^m = \delta_i^a - \frac{1}{6} (R^a_{iml} + R^a_{mil}) x^l x^m = \delta_i^a - \frac{1}{6} R^a_{mil} x^l x^m.
\end{align*}

The affine connection components are

\begin{align*}
  \Gamma^\mu_{0\nu} &= \Gamma^\mu_{\epsilon 0} = \frac{0}{0} R^\mu_{\nu 0} x^l, \\
  \Gamma^\mu_{ij} &= \frac{1}{3} (R^\mu_{ijl} + R^\mu_{jil}) x^l,
\end{align*}

where we are working to first order in $R^\mu_{\nu \lambda \rho}$. Using Eq. (3), the spinor connection components are found to be

\begin{align*}
  \omega_0 &= -\frac{1}{2} \gamma_0 \gamma_i R^0_{i 0l} x^l - \frac{1}{4} \gamma_i \gamma_j R^0_{ij} x^l, \\
  \omega_k &= -\frac{1}{4} \gamma_0 \gamma_i R^0_{k i 0} x^l - \frac{1}{8} \gamma_i \gamma_j R^0_{k j} x^l,
\end{align*}

working to first order in $R^\mu_{\nu \lambda \rho}$.

We find that all above formulas have the same form as those in the Fermi normal coordinates, if the gravitational field is chosen static. This can be regarded as a kind of equivalence between Riemann normal coordinates and Fermi normal coordinates.

**IV. RIEMANN TENSOR IN RIEMANN NORMAL COORDINATES WITH SCHWARZSCHILD GEOMETRY**

In Sec. III we find in Riemann normal coordinates that all physical quantities are expressed by the Riemann tensor at the origin point $p_0$. So it is necessary to get the expression of the Riemann tensor $R^\mu_{\nu \lambda \rho}$ in this coordinates. Therefore, we need another coordinates...
to describe the external gravitational field. In Schwarzschild coordinates, which we will call $X^\mu'$ or $cT, R, \Theta, \Phi$, the metric components $g_{\mu'\nu'}$ are displayed in the term

$$ds^2 = -g_{\mu'\nu'}dX^{\mu'}dX^{\nu'} = c^2XdT^2 - \frac{1}{X}dR^2 - R^2d\Theta^2 - R^2\sin^2\Theta d\Phi^2,$$

where $X = 1 - R_S/R$, $R_S = 2GM/c^2$ is the Schwarzschild radius, $M$ is the mass of the gravitation source.

The next step in constructing Riemann normal coordinates is to choose an orthonormal frame at the point $p_0$. The timelike base vector must be the tangent $\partial/\partial t$, and the symmetry determines the others. Conveniently we choose

$$\vec{e}_0 = \partial/\partial t = 1/\sqrt{X} \partial/\partial T,$$

$$\vec{e}_1 = \partial/\partial x = \sqrt{X} \partial/\partial R,$$

$$\vec{e}_2 = \partial/\partial y = 1/R \partial/\partial \Theta,$$

$$\vec{e}_3 = \partial/\partial z = 1/(R \sin \Phi) \partial/\partial \Phi.$$  

(20)

Where $x, y, z, t$ are the Riemann normal coordinates. We can compute the curvatures in the Riemann frame by the tensor transformation law

$$R_{abcd} = R_{\mu'\nu'\lambda'\rho'}e_\alpha^{\mu'}e_\beta^{\nu'}e_\gamma^{\lambda'}e_\delta^{\rho'}. $$

(21)

The curvature components $R_{\mu'\nu'\lambda'\rho'}$ with respect to the Schwarzschild frame are well known as

$$R_{1'0'1'0'} = R_S/R^3, \quad R_{2'0'2'0'} = -R_SX/(2R), $$

$$R_{3'0'3'0'} = -R_SX \sin^2\Theta/(2R), \quad R_{4'2'1'2'} = R_S/(2RX), $$

$$R_{2'3'2'3'} = R_SR \sin^2\Theta, \quad R_{1'3'1'3'} = R_S \sin^2\Theta/(2XR). $$

(22)

Only the independent non-vanishing components are listed above and below. From Eq. (20) we have

$$[e_\alpha^{\mu}] = \begin{pmatrix}
1/\sqrt{X} & 0 & 0 & 0 \\
0 & \sqrt{X} & 0 & 0 \\
0 & 0 & 1/R & 0 \\
0 & 0 & 0 & 1/(R \sin \Theta)
\end{pmatrix}.$$  

(23)
The computation then yields
\[
\begin{align*}
R_{1010} &= R_{S}R_{3}, \\
R_{1212} &= R_{1313} = \frac{R_{S}}{2R^3}, \\
R_{2020} &= R_{3030} = -\frac{R_{S}}{2R^3}, \\
R_{2323} &= -R_{S}R_{3}.
\end{align*}
\]
(24)

The above expressions of Riemann tensor have the same form with those in Fermi normal coordinates, which move along a radial geodesic[3, 7].

V. ENERGY-LEVEL SHIFTS IN THE SCHWARZSCHILD SPACETIME

Here we calculate the relativistic energy shifts of a hydrogen atom in the Schwarzschild spacetime. The exact solutions of the Dirac equation for a hydrogen atom in flat space-time serve as the basis for perturbation theory.

The energy eigenvalues of a hydrogen atom are
\[
E_{n\kappa} = mc^2/\sqrt{1 + \left(\frac{\zeta}{n - |\kappa| + s}\right)^2},
\]
(25)
where \(\zeta = Ze^2\), \(s = \sqrt{\kappa^2 - \zeta^2}\), \(m\) is the mass of electron, \(n = 1, 2, \cdots\) is the principal quantum number.

The bound state functions of a hydrogen atom can be written in standard representation as[10, 11, 12]
\[
\psi = \psi^{M}_{\kappa} = \begin{pmatrix} g(r)\chi^{M}_{\kappa} \\ -if(r)\chi^{-M}_{-\kappa} \end{pmatrix},
\]
(26)
here \(M\) and \(\kappa\) are the eigenvalues of \(J_z\) and \(K = b(\vec{\sigma} \cdot \vec{L} + I)\), respectively. The functions \(f(r)\), \(g(r)\) and spinors \(\chi^{M}_{\kappa}\), \(\chi^{-M}_{-\kappa}\) are given by
\[
f(r) = \frac{2^{s-\frac{1}{2}}\lambda^{s+\frac{3}{2}}}{\Gamma(2s+1)}\sqrt{\frac{\Gamma(2s+n_r+1)}{n_r!\zeta K_c(\zeta K_c - \lambda \kappa)}}\sqrt{1 - \frac{W_c r^{-s-1}e^{-\lambda r}}{K_c}} \\
\left(\left(\kappa - \frac{\zeta K_c}{\lambda}\right)F(-n_r, 2s + 1, 2\lambda r) - n_r F(-n_r + 1, 2s + 1, 2\lambda r)\right),
\]
(27)
\[
g(r) = -\frac{2^{s-\frac{1}{2}}\lambda^{s+\frac{3}{2}}}{\Gamma(2s+1)}\sqrt{\frac{\Gamma(2s+n_r+1)}{n_r!\zeta K_c(\zeta K_c - \lambda \kappa)}}\sqrt{1 - \frac{W_c r^{-s-1}e^{-\lambda r}}{K_c}} \\
\left(\left(\kappa - \frac{\zeta K_c}{\lambda}\right)F(-n_r, 2s + 1, 2\lambda r) + n_r F(-n_r + 1, 2s + 1, 2\lambda r)\right),
\]
(28)
\[ \chi^M_\kappa = C_{1/2} Y^M_{l-1/2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + C_{-1/2} Y^M_{l+1/2} \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad (29) \]

\[ \chi^M_{-\kappa} = -C_{1/2} Y^M_{l-1/2} \begin{pmatrix} \cos \theta \\ \sin \theta e^{i\phi} \end{pmatrix} - C_{-1/2} Y^M_{l+1/2} \begin{pmatrix} \sin \theta e^{-i\phi} \\ -\cos \theta \end{pmatrix}, \quad (30) \]

where \( W_c = E_{nm}/\hbar c, K_c = mc^2/\hbar c, \lambda = \sqrt{m^2c^4 - E^2_{nm}/\hbar^2 c}, \Gamma(2s + 1) \) is the \( \Gamma \) function, \( C_{1/2} \) and \( C_{-1/2} \) are the C-G coefficients.

The gravitational perturbation matrix elements are

\[ \langle H_I \rangle_{ij} \equiv (\psi_i, H_I \psi_j). \quad (31) \]

Also with the analyzing in Ref. [2], the perturbation Hamiltonian retaining the main term can be written as

\[ H_I = \frac{1}{2} \beta mc^2 \int_0^\theta x^l x^m. \quad (32) \]

Using the equation [2]

\[ \det[(\psi_i, H_I \psi_j) - E^1 \delta_{ij}] = 0, \quad (33) \]

and from the usual perturbation theory of a degenerate energy eigenvalue, the relativistic energy shifts of the atom we calculated can be found in Table II

VI. CONCLUSION

In this paper we investigate energy-level shifts of a stationary hydrogen atom in static external gravitational field. With the calculations we find the results in this case is same with a hydrogen atom freely falling along a radical geodesic [3]. From the results in Table II we find that the energy shifts of the states with total angular momentum quantum number \( \frac{1}{2} \) are zero, and the ratio of absolute energy shifts with total angular momentum quantum number \( \frac{5}{2} \) is 1 : 4 : 5. This feature can be used to help us to separate the shifts in the energy levels caused by other effects.
| State |
|-------|
| $1S_{1/2}$ |
| $2S_{1/2}$ |
| $2P_{1/2}$ |
| $2P_{3/2}$ |
| $3S_{1/2}$ |
| $3P_{1/2}$ |
| $3P_{3/2}$ |
| $3D_{3/2}$ |
| $3D_{5/2}$ |
| $4S_{1/2}$ |
| $4P_{1/2}$ |
| $4P_{3/2}$ |
| $4D_{3/2}$ |
| $4D_{5/2}$ |
| $4F_{5/2}$ |

**TABLE I: The energy-level shifts**

| State |
|-------|
| $1S_{1/2}$ |
| $2S_{1/2}$ |
| $2P_{1/2}$ |
| $2P_{3/2}$ |
| $3S_{1/2}$ |
| $3P_{1/2}$ |
| $3P_{3/2}$ |
| $3D_{3/2}$ |
| $3D_{5/2}$ |
| $4S_{1/2}$ |
| $4P_{1/2}$ |
| $4P_{3/2}$ |
| $4D_{3/2}$ |
| $4D_{5/2}$ |
| $4F_{5/2}$ |

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