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ON THE HYDROGEN ATOM IN KERR SPACE-TIME

BY A. K. GORBATSIEVICH

Department of Physics, Byelorussian State University, 220080 Minsk, USSR

AND A. PRIEBE

Central Institute for Astrophysics, Academy of Sciences of the GDR, Potsdam 1561, GDR

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The hydrogen atom is considered at the level of traditional quantum mechanics. Starting from a two-component Hamilton operator describing the atomic electron in the presence of an external gravitational field we are evaluating explicit expressions for the perturbations (i.e. splitting) of the energy levels. We restrict our considerations to geodesics on which $\theta = \pi/2$ and to "conical spiral" trajectories. It is shown that the perturbations can reach observable values for a sufficiently high initial velocity at inifinity.

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1. Introduction

Contrary to the situation in quantum field theory only a few papers deal with quantum mechanics in general relativity (see e.g. [1–6]). Most of them start from the generally covariant Dirac equation and rewrite it as a Schroedinger-type equation[1]:

$$i\hbar \frac{\partial \Psi}{\partial \tau} = H\Psi, \tag{1}$$

where τ is a parameter which represents the time (often proper time) and the operator H is interpreted as the energy operator, assuming that both time-evolution and energy are given by H. Such a procedure leads, in general, to a non-hermitean operator and other difficulties, which do not allow a simple physical interpretation of equation (1) (cf. e.g. [2–4, 7]). A detailed discussion of these problems by one of the authors (see [3, 5, 8] and references cited there) showed that it is always possible to treat the generally covariant Dirac equation as a special representation of the usual quantum evolution equation in

[1] Latin indices run from 1 to 4, Greek ones from 1 to 3. The signature of space-time is $(+, +, +, -)$. We will use (except of some starting equations and final results) units $c = \hbar = 1$.

a certain Hilbert space, and with a certain Hamilton operator, if one uses non-orthogonal basis vectors. A correct procedure was given to evaluate the Hamilton operator (whose expectation value in a quasistationary state is the energy corresponding to this state) for an electron of an (arbitrary moving) atom in an external gravitational and electromagnetic field. The atom is considered in the "frame of the single observer" (see e.g. [9]), which is given by the world line $\xi^i(\tau)$ of a point particle ("observer") — in the case considered here — the nucleus. Along this world line a comoving, i.e.

$$h^i_{(4)} = u^i := \frac{d\xi^i(\tau)}{d\tau} \qquad (2)$$

and orthonormal vierbein $h^i_{(j)}$ is introduced. This leaves three parameters free, which can be expressed for example in terms of the (three-) angular velocity of the vierbein:

$$\Omega^{(\alpha)} := \tfrac{1}{2}\, e^{(\alpha)(\beta)(\mu)} h^n_{(\mu)} h_{n(\beta);k} u^k. \qquad (3)$$

By introduction of three scalars $X^{(\alpha)}$ (a generalization of the Fermi coordinates to the case $\Omega \neq 0$) and restriction to a certain neighbourhood of the world line $\xi^i(\tau)$ of the nucleus one can get an explicit expression for the Hamilton operator H (For more details see [7, 8]).

In this paper we consider the freely falling hydrogen atom in the gravitational field of a rotating black hole, described by the Kerr metric (see Sect. 3). First we introduce the explicit expression for the two-component Hamilton operator, which is derived from the generally relativistic Dirac equation, then we summarize some properties of geodesics, which will be useful in the discussion of the Hamilton operator of an hydrogen atom in the Kerr space-time.

2. *Explicit expression for the Hamilton operator*

The two-component formulation of the generally covariant Dirac equation yields (in the absence of external electromagnetic fields) the following expression for the Hamilton operator of the atomic electron [3]:

$$H = H_0 + H_{RZ} + H_W + H_{GS}. \qquad (4)$$

This will be the basic equation for our analysis of quantum mechanics of the hydrogen atom in the Kerr space-time. H_0 is the operator of the non-perturbed hydrogen atom

$$H_0 = \frac{P^2_{(\alpha)}}{2m_e} - \frac{e^2}{4\pi\varepsilon_0 R} + H_F, \qquad (5)$$

where $R = (X^{(\alpha)}X_{(\alpha)})^{1/2}$, and H_F being the operator that gives the fine-structure splitting. The operators H_{RZ}, H_W and H_{GS} represent additional terms, which we assume to be small perturbations compared with H_0.

The operator H_W is due to the acceleration $w^{(\alpha)}$ of the frame. It was shown by one of the authors that for a freely falling atom the motion is indeed geodesic in a very good approximation [10], so that in this case we have $w^{(\alpha)} \equiv 0$. Therefore we will not discuss the term H_W. An example of effects in the hydrogen atom, caused by acceleration of the atom is discussed in detail in [11].

The operator H_{RZ}

$$H_{RZ} = -\Omega^{(\alpha)} J_{(\alpha)} \tag{6}$$

describes the influence of the rotation of the frame on the atomic electron. $J_{(\alpha)} = L_{(\alpha)} + \hbar/2\sigma_{(\alpha)}$ is the total momentum operator. The operator H_{RZ} has some analogy to the operator, which causes the (magnetic) Zeeman effect. Note that a rotation of the frame is in general necessary to guarantee the existence of quasistationary states of the electron. The operator H_{RZ} leads to a shift of the energy:

$$\Delta E_{RZ} = -\Omega(m_l + m_s), \tag{7}$$

where m_l and m_s are the quantum numbers of the projections of the operators of the orbital momentum and spin of the electron to $\Omega^{(\alpha)}$, Ω is the module of $\Omega^{(\alpha)}$ ($\Omega = (\Omega^{(\alpha)}\Omega_{(\alpha)})^{1/2}$). The shift ΔE_{RZ} yields a splitting of spectral lines into three components (in full analogy to the so-called "normal" Zeeman effect).

The operator

$$H_{GS} = \tfrac{1}{2}\, m_e c^2 R_{(4)(\alpha)(4)(\beta)} X^{(\alpha)} X^{(\beta)} \tag{8}$$

describes the direct influence of the external gravitational field to the atomic electron. $R_{(4)(\alpha)(4)(\beta)}$ are vierbein components of the curvature tensor.

The operator H_{GS} is on one hand a generalization of the classical tidal forces, which are represented by the tensor $R_{ikjl}u^i u^j$ in the equation for the geodesic deviation, and on the other hand a generalization of the usual electric Stark effect to the spin-two gravitational field, i.e. the latter depends quadratically on the "position operator" $X^{(\alpha)}$.

A similar formulation for the Hamilton operator of the electron in a gravitational field was given by L. Parker, although he assumed nonrotating frames ($\Omega = 0$) and geodesic motion of the atom only. In contrast, the power of the formalism, described in [7, 8] lies in the rigorous solution of the problems with the non-hermitean Hamilton operator and the definition of the scalar product of the wave function of the electron, while in the papers [1, 2, 4] the generally covariant Dirac equation is used only in a formal sense as a purely "mathematical equation".

We note that it is easy to include external electromagnetic fields into the formalism, so that it is possible e.g. to study the hydrogen atom in the field of a magnetic massive dipole (see [6]).

We will now summarize some features of certain geodesic trajectories in the Kerrs space-time, which will play a central role in the following discussion.

3. Geodesics with θ = const in the Kerr space-time

Let us first give a brief review of some notations for the Kerr metric. We consider the Kerr metric in Boyer-Lindquist coordinates (r, θ, φ, t):

$$ds^2 = \varrho^2\left(\frac{dr^2}{\Delta}+d\theta^2\right)+\left(r^2+a^2+\frac{1}{\varrho^2}a^2\sin^2\theta\right)\sin^2\theta d\varphi^2$$

$$-\frac{4Mra}{\varrho^2}\sin^2\theta d\varphi dt-\left(1-\frac{2Mr}{\varrho^2}\right)dt^2, \tag{9}$$

where

$$\varrho^2 = r^2+a^2\cos^2\theta, \quad \Delta = r^2-2Mr+a^2. \tag{10}$$

One determines the first integrals of the geodesic equation easily from the Hamilton--Jacobi equation (cf. [12]). In Boyer–Lindquist coordinates we get

$$(\varrho^2 u^r)^2 = P^2-\Delta(K+r^2),$$

$$(\varrho^2 u^\theta)^2 = K-(D^2+a^2\cos^2\theta),$$

$$\varrho^2 u^\varphi = \frac{a}{\Delta}P-\frac{D}{\sin\theta},$$

$$\varrho^2 u^t = \frac{r^2+a^2}{\Delta}P-a\sin\theta, \tag{11}$$

with

$$P(r) = \frac{1}{\mu}[E(r^2+a^2)-L_z a], \quad D(\theta) = \frac{1}{\mu}\left[Ea\sin\theta-\frac{L_z}{\sin\theta}\right]. \tag{12}$$

Here μ is the mass of the point mass (in our case the nucleus), E and L_z are the two well--known integrals of motion, corresponding to stationarity and axisymmetry of the Kerr solution of the Einstein equations. The quantity K is an integral of motion, which arises from the separation of variables in the Hamilton–Jacobi equation.

Furthermore we restrict our considerations to geodesics on the "cone" θ = const. This includes two important and interesting subcases:

(*i*) the motion in the equatorial plane ($\theta = \pi/2$), and

(*ii*) the motion along conical spirals ($\theta \neq \pi/2$),

and simplifies the calculations sufficiently.

The assumption θ = const has as a consequence the following condition (see [13]):

$$\frac{Du^\theta}{D\tau} \equiv -\frac{\mathrm{ctg}\,\theta}{\varrho^6}(\varrho^2 a^2\sin^2\theta-2a\sin\theta DP+(r^2+a^2+a^2\sin\theta)D^2) = 0. \tag{13}$$

For an atom moving in the equatorial plane Eq. (13) is fulfilled identically. On conical spirals, it can be rewritten as follows

$$E^2 = \mu^2 + \left(\frac{L_z}{a \sin^2 \theta}\right)^2. \tag{14}$$

As we consider only infinite motion of the atom, we introduce the velocity at infinity v_∞ and a generalized impact parameter l_0 by

$$\frac{E}{\mu} = \gamma \equiv (1 - v_\infty)^{-1/2}, \quad L_z = \mu \gamma v_\infty l_0 \sin \theta. \tag{15}$$

Then condition (10) reads

$$l_0 = \pm a \sin \theta \tag{16}$$

so that l_0 is (up to the sign) determined by a and θ. According to the sign of L_z (we assume $a > 0$), we have to distinguish two principally different cases of motion:

(*i*) $L_z < 0$: retrograde motion, and

(*ii*) $L_z > 0$: prograde motion.

It is favourable to express the quantity D (Eq. (12)) in terms of v_∞ and θ, which yields [7]

$$D_\pm = a \sin \theta \left(\frac{1 \mp v_\infty}{1 \pm v_\infty}\right)^{1/2} = \text{const}, \tag{17}$$

where upper signs belong to prograde motion. From Eq. (17) it follows immediately that the motion on conical spirals is essentially asymmetric, accordings to the sign of L_z. This asymmetry is marked out by the fact that it is *complete* in the sense that the ranges for $D_\pm(v_\infty)$ do not intersect for different signs of L_z:

$$0 < D_+ < a \sin \theta < D_- < \infty. \tag{18}$$

An important conclusion from this fact is discussed later. Note that the conical spiral trajectories are stable for small variations δE and δL_z [13].

Along the atoms trajectory we choose the comoving (cf. Eq. (2)) orthonormal vierbein $h^i_{(n)}$ in that way that it reflects maximally the symmetry of both the trajectory and the given motion, e.g. in our case $h^i_{(2)}$ will be parallel to the vector ∂_θ and $h^i_{(3)}$ has only one spacelike coordinate component (along ∂_φ). These conditions define the vierbein $h^i_{(n)}$ completely and allow to calculate explicit expressions for $\Omega^{(\alpha)}$ and $R_{(i)(j)(k)(l)}$ [7]. We will not write down these explicit expressions and mention only that no singularities occur outside the horizon.

4. *Hamilton operator in the Kerr field. Observable effects*

In what follows, we give explicit expressions for the shift and the splitting of the energy levels. It will be shown that large effects occur only for ultrarelativistically moving atoms, i.e

$$\gamma \gg 1, \tag{19}$$

where γ is the so-called Lorentz factor, introduced by Eq. (15). This allows us to express the results in a power series of γ and take into account only the highest order of the Lorentz factor. Hereby special attention is paid to those effects which are (at least in principle) accessible to modern experimental technique. It can be shown that although the Hamilton operator explicitly depends on τ, practically for all of the interesting trajecttories (including those regarded in the present paper) the gravitational field does not disturb the existence of quasistationary energy levels, i.e. the following inequality holds:

$$\frac{1}{\omega_{\mathrm{fi}}} \frac{d}{d\tau} |\langle \mathrm{i}| H(\tau) |\mathrm{f}\rangle| \ll \hbar\omega_{\mathrm{fi}}. \tag{20}$$

Here i and f indicate the initial and the final states correspondingly. Therefore the operators H_{GS} and H_{RZ} are regarded as corrections in the framework of Schroedinger's perturbation theory. We assume that the perturbations caused by these operators are greater than the fine-structure splitting, in order to simplify calculations. This consideration is not of principle importance. Explicit expressions for the energy splitting in the case of perturbations smaller than the fine-structure splitting (but greater than the hyperfine-splitting) are also easily obtained.

4.1. Motion in the equatorial plane

For motion in the equatorial plane the angular velocity has only one non-zero component:

$$\Omega = \Omega^{(2)} = \frac{1}{A^2\varrho^4}((r^2-3Mr+2a^2)DP - a(P^2+\Delta D^2)), \tag{21}$$

where $A^2 := 1/\varrho(P^2-\Delta D^2)^{1/2}$ has no singularities outside the horizon. The discussion of Eq. (21) and the explicit expression of the vierbein components $R_{(4)(\alpha)(4)(\beta)}$ (most favourably calculated in the Newman-Penrose formalism) shows that sufficiently large effects occur only for

$$\left|\frac{D}{r}\right| \gg 1, \tag{22}$$

i.e.

$$|a - v_\infty l_0| \gg 1 \tag{23}$$

and

$$l_0 \neq a. \tag{24}$$

This means that important effects occur if the atom is nearby the black hole and is moving ultrarelativistically. In the ultrarelativistic limit we get:

$$H_{\mathrm{GS}} = \tfrac{3}{2}\frac{M}{r^5}(l_0-a)^2[(X^{(2)})^2-(X^{(3)})^2]m_e c^2\gamma^2 \tag{25}$$

and

$$\Omega = \frac{1}{r^2}\left\{\frac{(r^2-al_0+a^2)(l_0-a)(r^2-3Mr+2a^2)}{(r^2-al_0+a^2)^2-\Delta(l_0-a)^2} + a\,\frac{(r^2-al_0+a^2)+\Delta(l_0-a)^2}{(r^2-al_0+a^2)-\Delta(l_0-a)^2}\right\}. \tag{26}$$

This yields

$$\frac{\langle H_{\rm GS}\rangle}{\langle H_{\rm RZ}\rangle} = \tfrac{3}{2}\,\alpha^{-1}\,\frac{M}{r}\,\frac{l_0-a}{r}\,\frac{R_{\rm B}}{r}\,n^4\gamma^2 = \delta, \tag{27}$$

where $\alpha \approx 1/137$ is Sommerfeld's fine-structure constant and $R_{\rm B} = 5.29\cdot 10^{-11}$ m, the Bohr radius of the hydrogen atom. Eq. (27) allows us to consider two limiting cases, for which we can give explicit results in a simple form:

(*i*) Dominance of gravitation: $\delta \gg 1$

If we suppose that M, a and r have the same order of magnitude, this case is equivalent to

$$r \ll n^4\gamma^2 R_{\rm B}. \tag{28}$$

The explicit expressions for the energy level shift for levels $n = 1$ and $n = 2$ are

$$\Delta E_{\rm GS}(n=1) = 0,$$

$$\Delta E_{\rm GS}(n=2) = \frac{18M}{r}\left(\frac{l_0-a}{r}\right)^2\left(\frac{R_{\rm B}}{r}\right) m_e c^2\gamma^2 m_l. \tag{29}$$

The expressions for higher n are much more complicated (cf. the results of Parker [4]).

(*ii*) Dominance of rotational effects: $\delta \ll 1$

This case holds if

$$r \gg n^4\gamma^2 R_{\rm B} \tag{30}$$

and the shifts of the energy levels are given by

$$\Delta E_{\rm RZ} = \hbar\Omega(m_l+m_s), \tag{31}$$

with the angular velocity given by Eq. (26). Note that the first order contribution to $\Delta E_{\rm RZ}$ does not depend on the Lorentz factor. The Schwarzschild limit of Eq. (26) leads to:

$$\Delta E_{\rm RZ}^{\rm Schw} = \frac{\hbar c m l_0}{r^2}\,\frac{1-\dfrac{3M}{r}}{1-\left(1-\dfrac{2M}{r}\right)\left(\dfrac{l_0}{r}\right)^2}. \tag{32}$$

This expression vanishes for radial trajectories ($l_0 = 0$) and on the photon sphere ($r = 3M$). The latter is obviously connected with our use of the ultrarelativistic approximation (Eq. (19)). The results (31) and (32) agree with [3, 5] where the atom in the field of a Schwarzschild black hole was considered (cf. also the expressions for ΔE for radially falling atoms in [1, 4]).

4.2. Motion on conical spirals

As in the case of motion in the equatorial plane, large effects occur only if condition (22) holds. This together with Eq. (18) suggests what we have to suppose to get sufficiently large perturbations:

(*i*) The atom is sufficiently nearby the Kerr black hole.
(*ii*) The atom moves ultrarelativistically: $\gamma \gg 1$.
(*iii*) The motion of the atom is retrograde, i.e. $L_z < 0$.

Note that according to Eq. (18) large effects, even for ultrarelativistically moving atoms, do not occur for prograde motion. This is caused by the (complete) asymmetry, discussed in Sect. 3.

Using the explicit expressions for $\Omega_{(\alpha)}$ and the vierbein components of the curvature tensor, we get:

$$\frac{\langle H_{GS}\rangle}{\langle H_{RZ}\rangle} = 3\alpha^{-1}\frac{M}{r}\frac{R_B}{r}\operatorname{tg}\theta n^4 \ll 1, \tag{33}$$

so that we can omit the operator H_{GS} when considering atoms falling along conical spirals.

Schroedinger's perturbation theory yields (in the ultrarelativistic approximation) the following expression for the shift of the energy levels:

$$\Delta E_{RZ} = \hbar c\,\frac{a^2 \sin 2\theta}{\Delta \varrho}\left(1+\frac{8Mr}{\varrho^2}\,\frac{a^2\sin^2\theta}{\varrho^2}\right)\gamma^2(m_l+m_s). \tag{34}$$

Note that the quantity ΔE_{RZ} does not depend on the parameters characterizing the atom and does not vanish on the ergosphere $r_{erg} = M+(M^2-a^2\cos^2\theta)^{1/2}$.

6. Conclusions

To give a more obvious representation of our results, let us make some numerical estimations. We will use M as a free parameter, characterizing the scale of the system, and set for definitness $r = 3M$, $a = 1/2M$. For motion in the equatorial plane we set $l_0 = 3M$ and consider conical spirals with $\theta = \pi/4$.

Thus we obtain the following values for the energy shift ΔE: For conical spirals the rotational Zeeman effect gives a splitting of order 10^{-11} eV$(M_S/M)\gamma^2$, where M_S is the mass of the Sun. That means that γ has to be of order 10^5 $(M/M_S)^{-1}$ to obtain effects of the order of the fine structure splitting. For motion in the equatorial plane we have $3\cdot 10^{-22}$ eV $(M/M_S)^{-2}\gamma^2$ for high γ and $2\cdot 10^{-11}$ eV $(M/M_S)^{-1}$ for low γ.

It seems to be possible, that near black holes or compact objects there are such atoms which have very large Lorentz factors so that the effects considered in this paper (especially those for conical spirals) really could be observed by astronomers. Actually, we should not forget that in addition to the splitting of energy levels and spectral lines, we have a systematic red-shift of the spectrum (in the ultrarelativistic approximation of order (1..10) γ), possibly up into the radio range. The obtained results let us hope contrary to the results of earlier papers, which dealt with non-moving atoms [1] that our results are not only of theoretical interest. Of course the established model is only a rough first approximation of more realistic ones, which should include an analysis of the mechanism of emission of photons (using QED), as well as ensembles of hydrogen atoms.

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