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ON THE EQUATION OF MOTION OF A ONE-ELECTRON ATOM IN AN EXTERNAL GRAVITATIONAL FIELD

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It is shown that the motion of an atom is given in a good approximation by Mathisson--Papapetrou equations if we put as a classical angular momentum of the atom the expectation value of the operator of the full angular momentum (including nuclear and electron spins an orbital momentum of the electron).

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1. *Introduction*

There are two main reasons for interest in the problem of atom motion in external gravitational fields: first — an atom is an extended quantum system with inner structure (for motion of extended bodies in general relativity see e.g. [1]), second — the knowledge of the law motion for the atomic systems is necessary to account influences of gravitational fields on atomic spectra. This, indeed, will become critical only in extremely strong gravitational fields with characteristic radii of curvature $\lesssim 10^{-3}$ cm [2], or in not very strong gravitational fields, e.g. outer range of macroscopic black holes with $r_g \gtrsim 10^5$ cm, but for ultrarelativistic motion of atoms [3]. Apparently, in both cases the motion of an atom cannot be considered a priori as a geodesic one. Subsequently we shall assume an atom with quasistationary quantum states.

Because of the negligible mass ratio of electron mass m and nucleus mass μ the motion of a classical mass point will be a good approximation for the motion of the nucleus $x^i = \xi^i(\tau)$, where τ is the proper time $(d\tau^2 = c^{-2}\, ds^2)$[1]. The motion of the electron is described by quantum mechanics, assuming only one-electron atom for simplification. Moreover, the assumed identity of atom and nucleus masses permits the consideration of the atomic motion as a nuclear one. One can obtain the equation for $\xi^i(\tau)$ from the following suggested model.

[1] Latin indices run from 1 to 4, Greek ones from 1 to 3. The signature of the space-time metric is $(+, +, +, -)$.

The nucleus, in the classical mass-point approximation with intrinsic spin, is moving in an external gravitational field and interacting with the electromagnetic field of the electron. The electron which for his part is moving in the external gravitational field and in the nuclear electromagnetic field, is considered in a quasistationary bound quantum state. It was shown by different authors [4] that the expectation values of the position and spin operators for a Dirac electron fulfil Mathisson-Papapetrou equations. Applying these results (valid for any Dirac particles) to the nucleus, we describe its motion in our model by the system of Mathisson-Papapetrou equations [5]. To the first equation of this system we have to add a "Lorentz-force" term which describes in first approximation the interaction with mean electromagnetic field of the electron. This leads us to[2]

$$\mu \frac{Du^i}{D\tau} = \frac{1}{2c} R^i{}_{bcd} u^b \varepsilon^{cdpq} \bar{S}_p u_q + \frac{q}{c} F^{ij} u_j, \tag{1a}$$

$$\frac{D\bar{S}^i}{D\tau} = \frac{1}{c^2} u^i \bar{S}_n \frac{Du^n}{D\tau}, \qquad u^n \bar{S}_n = 0, \tag{1b}$$

where q, $u^i = d\xi^i/d\tau$, and $\bar{S}^i$ denote the charge, the 4-velocity and the classical spin of the nucleus respectively. We shall regard the expectation value of the nuclear spin operator as classical spin. ε^{ijmn} denotes the Levi-Civita pseudotensor with $\varepsilon^{1234} = (-g)^{-1/2}$ and $g = \det(g_{ij})$, $R^i{}_{klm}$ is the Riemann curvature tensor and F^{ij} is the tensor of the electromagnetic field of the electron. Here, we have only to calculate the tensor F^{ij} to obtain an equation for $\xi^i(\tau)$. In order to simplify calculations we shall deal with a special, comoving reference frame.

2. *Choice of the reference frame*

We use the frame of the single observer [7] as a comoving one. This reference frame is determined by the motion of a single mass point. The world line of this mass point ("single observer") is named basis. Using the world line $\xi^i(\tau)$ of the nucleus as basis, we obtain a convenient comoving reference frame for the atom. Along the basic line we establish an orthonormal vierbein $h_{(m)}{}^i$, defined by $h_{(4)}{}^i = \frac{1}{c} u^i$. The introduced vierbein is determined with exception of three-dimensional rotations. The three-dimensional physical space is given by a geodesic spacelike hypersurface f (related to τ), which lies orthogonal to the basic world line. In order to arithmetize the hypersurface f, at each point $P \in f$ we fix a set of three scalars $X^{(\alpha)} = \sigma_P h^{(\alpha)}{}_i k^i$, where σ_P is the value of the canonic parameter σ at P, defined along a spacelike geodesic in f and going through the point P, k^i is the tangent unit vector to that geodesic, defined at the point on the basic line ($\sigma = 0$).

[2] We neglect $-c^{-3}\varepsilon^{arq}{}_p \bar{S}_r u_q \frac{D^2u^p}{D\tau^2}$, and also terms which describe interaction between the field F^{ij} and the nuclear magnetic momentum (these terms can be found in [6]). Numerical calculations show that they are smaller than all other terms in (1).

For a nonrotating frame (i.e. the vectors $h_{(n)}{}^{i}$ are displaced along the basic line $\xi^{i}(\tau)$ according to the Fermi-Walker transport) the quantities $((X^{(\alpha)}, c\tau)$ correspond to the Fermi normal coordinates [8]. Analogous quantities $X^{\hat{\alpha}} = X^{(\alpha)}$, $X^{\hat{4}} = c\tau$ we treat as rotating Fermi coordinates. In these coordinates the metric tensor $g_{\hat{i}\hat{j}}$ becomes

$$g_{\hat{i}\hat{j}} = \eta_{(i)(j)} + \varepsilon_{(i)(j)}, \tag{2}$$

with $\eta_{(i)(j)} = \operatorname{diag}(1, 1, 1, -1)$ being the Minkowski tensor and

$$\varepsilon_{(\alpha)(\beta)} = -\tfrac{1}{3} R_{(\alpha)(\mu)(\beta)(\nu)} X^{(\mu)} X^{(\nu)} + O(\varrho^{3}), \tag{3a}$$

$$\varepsilon_{(\alpha)(4)} = \frac{1}{c}\, e_{(\alpha)(\kappa)(\tau)} X^{(\tau)} \omega^{(\kappa)} + \theta_{(\alpha)}, \tag{3b}$$

$$\varepsilon_{(4)(4)} = -2\left(\theta + \frac{1}{c^{2}}\, W_{(\alpha)} X^{(\alpha)}\right); \tag{3c}$$

$$\theta_{(\alpha)} = \tfrac{2}{3} R_{(\alpha)(\mu)(\nu)(4)} X^{(\mu)} X^{(\nu)} + O(\varrho^{3}), \tag{4a}$$

$$\theta = \tfrac{1}{2}\left(R_{(4)(\mu)(4)(\nu)} - \tfrac{1}{2} R_{(4)(\mu)(4)(\nu)(\tau)} X^{(\tau)}\right) X^{(\mu)} X^{(\nu)} + O(\varrho^{4}). \tag{4b}$$

Here, we used the following notations: $W^{(\alpha)} = h^{(\alpha)}{}_{i} \dfrac{Du^{i}}{D\tau}$ and $\omega^{(\alpha)} = \tfrac{1}{2} e^{(\alpha)(\kappa)(\tau)} h_{(\tau)i} \dfrac{Dh_{(\kappa)}{}^{i}}{D\tau}$ are the acceleration and the angular velocity of the reference frame respectively, $e^{(\alpha)(\kappa)(\tau)}$ is the three-dimensional Levi-Civita symbol, $R^{(i)}{}_{(m)(n)(k)}$ and $R^{(i)}{}_{(m)(n)(k)(l)} = h^{(i)}{}_{a} h_{(m)}{}^{b} \times h_{(n)}{}^{c} h_{(k)}{}^{p} h_{(l)}{}^{r} R^{a}{}_{bcp;r}$ are the vierbein-components of the Riemann curvature tensor and of its covariant derivative respectively. Because $\varrho \equiv \sqrt{X_{(\alpha)} X^{(\alpha)}}$ is in order of the atomic radii, the condition $\varepsilon_{(i)(j)} \ll 1$ is valid even for extremely strong (from a macroscopic viewpoint) gravitational fields, and without much loss of accuracy one can keep only linear terms in the $\varepsilon_{(i)(j)}$. For further calculations we write down the system (1) in the rotating Fermi coordinates. From $u^{\hat{i}} = (0, 0, 0, c)$, $g_{\hat{i}\hat{j}}(0) = \eta_{(i)(j)}$, and $\left(\dfrac{\partial x^{i}}{\partial x^{\hat{j}}}\right)_{x=0} = h_{(j)}$ it follows that

$$\mu W_{(\nu)} = -c e^{(\mu)(\kappa)(\tau)} R_{(4)(\kappa)(\nu)(\mu)} \bar{S}_{(\tau)} + q F_{(\nu)(4)}, \tag{5a}$$

$$\frac{d}{d\tau} \bar{S}_{(\alpha)} = e_{(\alpha)(\kappa)(\nu)} \omega^{(\nu)} \bar{S}^{(\kappa)}, \qquad \bar{S}_{(4)} = 0. \tag{5b}$$

In equations (5) all quantities are taken along the basic line ($X^{(\alpha)} = 0$).

3. *Calculation of* $F_{(\alpha)(4)}$

We shall calculate the vierbein-components of the mean electromagnetic field at the point $X^{(\alpha)} = 0$, generated by the atomic electron in the following way: first, solving Maxwell equations we determine the field of a stationary point charge e, which is located at the point $X^{(\alpha)}$. After that, we calculate the expectation value of that field, using the assumption that the electron is in a quasistationary state, and neglecting both the interaction of the electron magnetic field with the nuclear magnetic momentum and the effects of the retardation. It is clear that those retardation effects will become small enough because of the small velocity of the electron within the atom ($v/c \ll 1$). By means of the Maxwell equations we find that in a certain neighbourhood of the nucleus the electromagnetic field will be quasistationary (for the same limitations as made above to the space-time metric and to the law of motion for the atom, which guarantee the existence of quasistationary states). At the point with the coordinates $\zeta^{(\alpha)}$ the electromagnetic field is given by

$$\varphi(\zeta^{(\alpha)}) = \frac{e}{R}\left[1 + \frac{1}{2c^2} W_{(\kappa)}R^{(\kappa)} + \tfrac{1}{3} R_{(4)(\kappa)(4)(\tau)}\zeta^{(\kappa)}(\zeta^{(\tau)} - \tfrac{1}{2} X^{(\tau)}) \right.$$
$$\left. + \frac{1}{6R^2} R_{(\kappa)(\tau)(\nu)(\mu)}\zeta^{(\kappa)}\zeta^{(\nu)}X^{(\tau)}X^{(\mu)} + O(\varrho^3)\right], \tag{6a}$$

$$A_{(\alpha)}(\zeta^{(\alpha)}) = \frac{e}{R}\left[- \frac{1}{c} e_{(\alpha)(\tau)(\nu)}X^{(\tau)}\omega^{(\nu)} + \tfrac{1}{6} R_{(4)(\tau)(\nu)(\alpha)}\zeta^{(\tau)}\zeta^{(\nu)} \right.$$
$$\left. + \tfrac{1}{2} R_{(4)(\alpha)(\tau)(\nu)}X^{(\tau)}\zeta^{(\nu)} + \tfrac{1}{2} R_{(4)(\nu)(\tau)(\alpha)}X^{(\nu)}X^{(\alpha)} + O(\varrho^3)\right] \tag{6b}$$

with $\varphi = -A_{\hat{4}}$, $A_{(\alpha)} = A^{(\alpha)} = A_{\hat{\alpha}}$ the scalar and vector potentials and $R^{(\alpha)} = \zeta^{(\alpha)} - X^{(\alpha)}$, $R \equiv \sqrt{R^{(\alpha)}R_{(\alpha)}}$. To deduce Eqs. (6) we assume that the gravitational field is a vacuum one (i.e. $R_{ij} = 0$) within the atom, a restriction which is always valid since the curvature appearing here is that of the background geometry, and not that generated by atom itself or by an external electromagnetic field. From Eqs. (6) we obtain the following expansions for the electromagnetic field tensor

$$F_{(\alpha)(4)} = \langle \hat{F}_{(\alpha)(4)} \rangle, \tag{7}$$

where

$$\hat{F}_{(\alpha)(4)} \cong -\left(\frac{\partial \varphi}{\partial \zeta^{(\alpha)}}\right)_{\zeta^{(\nu)}=0} \cong -\frac{eX_{(\alpha)}}{\varrho^3} - \frac{e}{\varrho}\left(\tfrac{1}{3} R_{(\alpha)(4)(4)(\tau)}X^{(\tau)} + \frac{1}{2c^2} W_{(\alpha)}\right). \tag{8}$$

In order to determine the expectation value in Eq. (7) we notice that the covariant Dirac equation can be interpreted as a special representation of the traditional quantum-mechanical law of motion in Hilbert space, which allows one to build quantum mechanics in arbitrary reference frames and under consideration of external gravitational fields [3] (for details see the book [9]). In particular, one can show that in quasirelativistic approximation the electron can be always described by a two-component Pauli-type equation

$$i\hbar \frac{\partial \varphi}{\partial \tau} = H\varphi \tag{9}$$

(with

$$\int_f \varphi^+ \varphi d^3X = 1, \tag{10}$$

and $d^3X = dX^{(1)}dX^{(2)}dX^{(3)}$) in the reference frame of a single observer. The complete expressions for the two-component Hamiltonian H one can find in the papers [3, 9] (see also [2]). A discussion of the complete operator H shows that the influence of external gravitational field will always be more significant than effects caused by the non-Coulomb participants of the nuclear potentials[3]. Therefore, in a good approximation the Hamiltonian is given by

$$H = H_0 + H_1, \tag{11}$$

with $H_0 = P^2/2m - qe/\varrho + O(1/c^2)$ — the Hamiltonian of a non-disturbed electron which is bound by a nucleus and H_1 describing the interaction with the external gravitational field

$$H_1 \cong mc^2\theta + \frac{c}{2}\left(e^{(\sigma)(\alpha)(\tau)}\theta_{(\sigma),(\alpha)}S_{(\tau)} - \{\theta^{(\alpha)}, P_{(\alpha)}\}\right)$$
$$-\omega^{(\alpha)}(L_{(\alpha)} + S_{(\alpha)}) + mW_{(\alpha)}X^{(\alpha)} + O(1/c^0). \tag{12}$$

In the last equation we introduced the following notations $P_{(\alpha)} = \frac{\hbar}{i}\,\partial/\partial X^{(\alpha)}$, $L_{(\alpha)} = e_{(\alpha)(\kappa)}{}^{(\tau)} \times X^{(\kappa)}P_{(\tau)}$, $S_{(\alpha)} = \frac{\hbar}{2}\sigma_{(\alpha)}$, where $\sigma_{(\alpha)}$ are the standard Pauli matrices.

As the states of a non-disturbed atom are either even or odd, we have

$$\langle \hat{F}_{(\alpha)(4)} \rangle_0 = -\frac{e}{2c^2} W_{(\alpha)} \langle 1/\varrho \rangle_0. \tag{13}$$

The notation $\langle \ldots \rangle_0$ means that the expectation values are calculated using eigenvectors of H_0. If one neglects "deformation" of the atom by gravitational field, $F_{(\alpha)(4)}$ will affect only renormalization of the mass of the nucleus $\mu \to \mu + \Delta\mu$ with $\Delta\mu = eq/2c^2a$, and $a = \langle \varrho \rangle_0$ being the radius of the atom. Because of $\Delta\mu/\mu \ll 1$, we shall not consider this renormalization. This means that we have to calculate only the expectation values with the eigenvectors of the full Hamiltonian H to determine $F_{(\alpha)(4)}$. Using perturbation theory one can show easily that

$$F_{(\alpha)(4)} = \langle -eX_{(\alpha)}/\varrho^3 \rangle + \text{terms quadratic in } \varepsilon_{(i)(j)}. \tag{14}$$

Direct calculation of $\langle -eX_{(\alpha)}/\varrho^3 \rangle$ is connected with several difficulties. Therefore we act as follows.

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[3] The electromagnetic potentials of the nucleus are obtained from Eqs. (6) by changing $e \to q$, $\zeta^{(\kappa)} \rightleftarrows X^{(\kappa)}$, and then $\zeta^{(\alpha)} \to 0$. Analogous results (without considering rotation and acceleration of the reference frame) were found by Parker [2], unfortunately, with some inaccuracy in the coefficient at $R_{(4)(\nu)(\mu)(4)}X^{(\nu)}X^{(\mu)}$ in the expression for φ.

If A is any Hermitean operator, the operator

$$\mathring{A} \equiv \left(\frac{\partial A}{\partial \tau}\right)_{\text{expl}} + \frac{i}{\hbar}[H, A] \tag{15}$$

will describe the observable "evolution of the observable A", since

$$\frac{d}{dt}\langle A\rangle = \langle \mathring{A}\rangle. \tag{16}$$

If, besides, A does not depend on time τ explicitly, the expectation value of $\mathring{A}$ in a stationary state (for which the state vector is an eigenvector of the Hamiltonian) will be identically equal to zero. In our case the Hamiltonian H_1 (12) generally depends explicitly on proper time τ along the basic line, because θ, $\theta_{(\alpha)}$ and both $\omega^{(\alpha)}$ and $W^{(\alpha)}$ depend on time. However, generally, the time dependence of the operator H will be sufficiently weak (except of gravitational shortwave radiation). Indeed, even if the motion of the nucleus is ultrarelativistic, the atom covers only a short distance during a characteristic atomic time ($\sim 10^{-5}$ cm). In these dimensions, gravitational fields are actually homogeneous. Direct calculation shows that atomic states will be quasistationary and that the following equations for the operators of the 3-velocity and 3-acceleration

$$\langle \mathring{x}^{(\alpha)}\rangle \cong 0, \quad \langle \mathring{\mathring{x}}^{(\alpha)}\rangle \cong 0 \tag{17}$$

will be a good approximation with high precision. Using explicit time-independence of the operators $X^{(\alpha)}$ and $P_{(\alpha)}$ and the fact that the "gravitational potentials" θ and $\theta_{(\alpha)}$ vary slowly with time, by means of the above equations one finds

$$\left\langle -\frac{eqX_{(\nu)}}{\varrho^3}\right\rangle \cong cR_{(\nu)(\kappa)(4)(\mu)}e^{(\mu)(\kappa)(\tau)}\langle L_{(\tau)}+S_{(\tau)}\rangle - mW_{(\nu)} - mc^2\langle\theta_{,(\nu)}\rangle. \tag{18}$$

Note that we made use of the equality

$$R_{(4)(\mu)(\kappa)(\nu)}\langle\{X^{((\mu)}, P^{(\nu))}\}\rangle \cong m\langle\mathring{\theta}_{(\kappa)}\rangle \cong 0. \tag{19}$$

By means of Eqs. (4) and (18), equation (5) leads (up to terms quadratic in $\varepsilon_{(i)(j)}$) to

$$(\mu+m)W_{(\nu)} = -cR_{(4)(\kappa)(\nu)(\mu)}[\bar{S}_{(\tau)}+\langle S_{(\tau)}+L_{(\tau)}\rangle_0]e^{(\mu)(\kappa)(\tau)}$$
$$+\tfrac{1}{4}mc^2[R_{(4)(\mu)(4)(\nu)(\tau)}+R_{(4)(\tau)(4)(\mu)(\nu)}+R_{(4)(\nu)(4)(\tau)(\mu)}]\langle X^{(\mu)}X^{(\nu)}\rangle_0, \tag{20}$$

where neglecting of quadratic terms in $\varepsilon_{(i)(j)}$ allowed us to change from $\langle\ldots\rangle$ to $\langle\ldots\rangle_0$. From estimations made above, it follows that the second term on the r.h.s. of Eq. (20) becomes actually small and negligible with regard to the atomic dimensions, if we assume that full spin of the atom (nuclear spin + electron spin + orbital angular momentum of the electron) is non-zero. The calculations of the expectation values of the operator

$\dot{L}_{(\alpha)}+\dot{S}_{(\alpha)}$ describing variation of the electron angular momentum, by means of Eq. (5b), lead us to

$$\frac{d}{d\tau}(\bar{S}_{(\alpha)}+\langle L_{(\alpha)}+S_{(\alpha)}\rangle) \cong e_{(\alpha)}{}^{(\nu)(\kappa)}\omega_{(\kappa)}(\bar{S}_{(\nu)}+\langle L_{(\nu)}+S_{(\nu)}\rangle_0). \tag{21}$$

In this way we demonstrated that the motion of an atom is given by Mathisson–Papapetrou equations in a good approximation if we put as a classical angular momentum the expectation value of the operator of the full angular momentum (including the nuclear and electron spins and the orbital angular momentum of the electron).

We note that the consideration of external electromagnetic field ${}^{(0)}F^{ij}$ yields additional terms

$$\frac{1}{c}(e+q)^{(0)}F^{ij}u_j+\frac{1}{c}F^{i}{}_{m;n}\varepsilon^{mnsp}M_s u_p \tag{22}$$

in Eq. (1a), where M_i is the 4-vector of the atoms full magnetic moment. Particularly in a comoving frame of reference one gets $M^{(4)}=0$, $M_{(\alpha)}=e/2mc\langle L_{(\alpha)}+2S_{(\alpha)}\rangle_0+(qg/2\mu c)\times\bar{S}_{(\alpha)}$.

Editorial note. This article was proofread by the editors only, not by the author.

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