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ATOMIC PHYSICS IN A GRAVITATIONAL FIELD

NOTES

(Not a polished presentation)

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In treating an atom in the strong gravitational field near a massive object, there are two basic issues: How does the field modify the Coulomb potential and how to do quantum mechanics in the modified potential. The first question can be answered by the standard methods of general relativity. In connection with the second, we propose to explore the proposal of Johnson (reference) for a unified algebraic approach to the formulation of quantum theory in the presence of gravity. In this approach, four-vector position and momentum operators for the electron satisfy commutation rules

$$[p^i, x^j] = i\hbar g^{ij} \tag{1}$$

defined by the local gravitational metric. (We follow here the general relativistic notation of Landau and Lifschitz' *Classical Theory of Fields* in which roman indices run from 0 to 3 and greek indices run from 1 to 3.) This gives rise to a local Lie algebra in which includes the Poincare group generators as well as the position operators (see Johnson). The ultimate objective is to find experimentally observable consequences of Johnson's proposal. This will be done first assuming the nucleus to have fixed Schwarzchild spatial coordinates.

Near a massive non-rotating spherical object, the metric is given by Schwarzchild to be

$$ds^2 = (1 - \frac{r_g}{r})c^2dt^2 - \frac{1}{1 - \frac{r_g}{r}}dr^2 - r^2d\Omega. \tag{2}$$

The Schwarzchild radius r_g is $2GM/c^2$ if M is the mass of the object and G is Newton's gravitational constant. Let the nucleus be located at the point $r = r_0$, $\theta = \pi/2$, and $\phi = 0$. An electron in this atom can be described by Cartesian nucleocentric coordinates (x, y, z), introduced via the relations

$$\begin{aligned} r^2 &= (r_0 + z)^2 + x^2 + y^2, \\ \tan\theta &= \frac{\sqrt{x^2 + y^2}}{r_0 + z}, \\ \tan\phi &= \frac{y}{x}. \end{aligned} \tag{3}$$

The atomic z-axis is oriented along a radial line from the center of the gravitating object. From these equations, the coordinate differentials can be obtained:

$$\begin{aligned} dr &= \frac{r_0 + z}{r} dz + \frac{x}{r} dx + \frac{y}{r} dy, \\ d\theta &= -\frac{\sqrt{x^2 + y^2}}{r^2} dz + \frac{r_0 + z}{r^2 \sqrt{x^2 + y^2}} (xdx + ydy), \\ d\phi &= \frac{1}{x^2 + y^2} (xdy - ydx). \end{aligned} \tag{4}$$

It is convenient to introduce the function $\beta(r) = r_g/(r - r_g)$, which is zero far from the source of gravitation and infinity at the event horizon. The Schwarzchild metric then takes the form:

$$ds^2 = \frac{c^2 dt^2}{1 + \beta} - \frac{\beta}{r^2} \left((r_0 + z)dz + xdx + ydy\right)^2 - dx^2 - dy^2 - dz^2. \tag{5}$$

(see A) Far from the gravitating mass this is the Minkowski metric. Though the metric is diagonal in the Minkowski limit, it becomes non-diagonal when β is non-zero. It does not seem necessary to redefine the Cartesian coordinates as a function of β to make the metric diagonal. The determinant of the space-time metric is $-g = 1$, the determinant of the spatial metric is $\gamma = |-g_{\alpha\beta}| = (1 + \beta)$, and the spatial part of the contravariant metric tensor is

$$[-g^{\alpha\beta}] = \frac{1}{1 + \beta} \begin{bmatrix} 1 + \beta\frac{r^2 - x^2}{r^2} & -\beta\frac{xy}{r^2} & -\beta\frac{x(r_0+z)}{r^2} \\ -\beta\frac{xy}{r^2} & 1 + \beta\frac{r^2 - y^2}{r^2} & -\beta\frac{y(r_0+z)}{r^2} \\ -\beta\frac{x(r_0+z)}{r^2} & -\beta\frac{y(r_0+z)}{r^2} & 1 + \beta\frac{r^2 - (r_0+z)^2}{r^2} \end{bmatrix}. \tag{6}$$

Starting from the equation for the electromagnetic field

$$\frac{1}{\sqrt{-g}}\frac{\partial}{\partial x^k}\left(\sqrt{-g}F^{ik}\right) = -4\pi j^i, \tag{7}$$

we introduce the four-vector potential A^i via

$$F^{ij} = A^{j;i} - A^{i;j} = \frac{\partial A^j}{\partial x_i} - \frac{\partial A^i}{\partial x_j} \tag{8}$$

(the added terms in the covariant derivatives cancel due to the symmetry properties of the affine connection) and specialize to the case of no magnetic field ($F^{\alpha\beta} = 0$, $A^\alpha = 0$) and time independent quantities to obtain Poisson's equation

$$\frac{1}{\sqrt{-g}}\frac{\partial\sqrt{-g}}{\partial x^\alpha}g^{\alpha\beta}\frac{\partial A^0}{\partial x^\beta} - g^{\alpha\beta}\frac{\partial^2 A^0}{\partial x^\alpha \partial x^\beta} = -4\pi j^0. \tag{9}$$

Since $-g = 1$ independent of the coordinates, only the second term on the left survives.

In writing Eq.(9) explicitly, it is useful to estimate the magnitudes of β and x/r_0 at the surface of typical massive objects. For example, a stellar black hole of 10 solar masses, a member of a binary, would have a Schwarzchild radius of 1.77×10^4 m. At this distance, x/r_0 can be estimated as the Bohr radius divided by the Schwarzchild radius a/r_g, which is of the order 10^{-14}. Due to the strengthening of the Coulomb potential in the gravitational field (see below) this would be reduced by a factor $1/(1+\beta)$, since $a = \hbar^2/me^2$ would be replaced by $a/(1+\beta)$. This has an infinitesimal value near the event horizon, where $\beta \to \infty$. At the surface of a neutron star of 3 solar masses with radius estimated as 1.5×10^4 m, the value of β would be 1.44 and the ratio of a to r_0 would still be of order 10^{-14}. This seems the most promising place to observe the effects of gravitation and modified quantum mechanics. However, the effects of the very large magnetic field (10^{11} gauss) would have to be accounted for. For comparison, at the surface of a typical white dwarf, β would be approximately 2×10^{-4}. In view of these estimates, it is a good approximation to take the spatial part of the contravariant metric tensor to be

$$[-g^{\alpha\beta}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \frac{1}{1+\beta} \end{bmatrix}, \tag{10}$$

and to take the value of β at the nucleus.

The charge density ρ is defined as the charge per unit physical volume, $\rho = dQ/\sqrt{\gamma}d^3V$, where d^3V is the spatial coordinate volume element. Noting that $\sqrt{-g}dx^0d^3V$ is the invariant 4-volume, we see that the current density

$$j^i = \frac{c\rho}{\sqrt{g_{00}}}\frac{dx^i}{dx^0} = \frac{cdQ}{\sqrt{-g}d^3V}\frac{dx^i}{dx^0} \tag{11}$$

is indeed a 4-vector, since the denominator and the coefficient of dx^i in the numerator are invariants. The right hand side of Eq.(9) is therefore $-4\pi c\rho/\sqrt{g_{00}} = -4\pi c\rho\sqrt{1+\beta}$. The charge density corresponding to a point charge can be expressed as a delta function of the spatial coordinates $A\delta^3(x^\alpha)$. To determine A, integrate this over a physical volume containing the charge Ze to obtain $\rho = Ze\delta^3(x^\alpha)/\sqrt{\gamma} = Ze\delta^3(x^\alpha)/\sqrt{1+\beta}$. Using Eq.(10), Poisson's equation then becomes

$$\frac{\partial^2 A^0}{\partial x^2} + \frac{\partial^2 A^0}{\partial y^2} + \frac{1}{1+\beta}\frac{\partial^2 A^0}{\partial z^2} = -4\pi Zec\delta^3(x^\alpha). \tag{12}$$

This equation can be solved by scaling the z coordinate by introducing $\zeta = z\sqrt{1+\beta}$. Eq,(12) becomes

$$\frac{\partial^2 A^0}{\partial x^2} + \frac{\partial^2 A^0}{\partial y^2} + \frac{\partial^2 A^0}{\partial \zeta^2} = -4\pi Zec\sqrt{1+\beta}\delta(x)\delta(y)\delta(\zeta). \tag{13}$$

This has the form of the Poisson equation in the variables (x, y, ζ) for a charge of magnitude $Ze\sqrt{1+\beta}$. The solution is therefore

$$A^0 = \frac{Zec\sqrt{1+\beta}}{\sqrt{x^2+y^2+\zeta^2}} \tag{14}$$

or, in terms of the original coordinates,

$$A^0 = \frac{Zec\sqrt{1+\beta}}{\sqrt{x^2+y^2+(1+\beta)z^2}}. \tag{15}$$

The Coulomb potential is thus increased by a factor $\sqrt{1+\beta}$ and compressed in the z direction by $1/\sqrt{1+\beta}$.

0.1 $2p \to 1s$ transition in hydrogenic atoms

As an example, we will treat the $2p \to 1s$ transition in a stationary, i.e., with constant Schwartzchild coordinates, hydrogenic atom. Consider first the modification of the spectrum due to the gravitational distortion of the Coulomb potential. First order degenerate perturbation theory will be accurate for a range of values of $\beta = r_g/(r - r_g)$. The perturbing potential is given by

$$V = -\frac{Ze^2}{r}\left[\frac{\sqrt{1+\beta}}{\sqrt{1+\beta\cos^2\theta}} - 1\right]. \tag{16}$$

Letting a denote the Bohr radius $\hbar^2/Zme^2$, the non-vanishing matrix elements of this perturbation between the four degenerate $2p$ states:

$$\begin{aligned}
\psi_{21m} &= \mp\left(\frac{1}{2a}\right)^{3/2}\frac{r}{a\sqrt{3}}e^{-r/2a}\sqrt{\frac{3}{8\pi}}\sin\theta e^{im\phi}, \\
\psi_{210} &= \left(\frac{1}{2a}\right)^{3/2}\frac{r}{a\sqrt{3}}e^{-r/2a}\sqrt{\frac{3}{4\pi}}\cos\theta \\
\psi_{200} &= \left(\frac{1}{2a}\right)^{3/2}\left(2-\frac{r}{a}\right)e^{-r/2a}\sqrt{\frac{1}{4\pi}}
\end{aligned} \tag{17}$$

can be evaluated in closed form:

$$\begin{aligned}
V_{21m,21m} &= -\frac{3Ze^2}{16a}\left[2\frac{\sqrt{1+\beta}}{\sqrt{\beta}}\sinh^{-1}\sqrt{\beta} - \frac{1+\beta}{\beta} + \frac{\sqrt{1+\beta}}{\beta\sqrt{\beta}}\sinh^{-1}\sqrt{\beta} - \frac{4}{3}\right], \\
V_{210,210} &= -\frac{3Ze^2}{8a}\left[\frac{1+\beta}{\beta} - \frac{\sqrt{1+\beta}}{\beta\sqrt{\beta}}\sinh^{-1}\sqrt{\beta} - \frac{2}{3}\right], \\
V_{200,200} &= -\frac{Ze^2}{4a}\left[\frac{\sqrt{1+\beta}}{\sqrt{\beta}}\sinh^{-1}\sqrt{\beta} - 1\right].
\end{aligned} \tag{18}$$

The matrix element of the perturbation in the $1s$ state

$$\psi_{100} = 2\left(\frac{1}{a}\right)^{3/2} e^{-r/a}\sqrt{\frac{1}{4\pi}} \tag{19}$$

is

$$V_{100,100} = -\frac{Ze^2}{a}\left(\frac{\sqrt{1+\beta}}{\sqrt{\beta}}\sinh\sqrt{\beta} - 1\right) \tag{20}$$

The effects of the modified commutation rule (1) can also, for a certain range of β, be treated via perturbation theory. According to the Eq.(10), the commutator $[p_z, z]$ is modified from $i\hbar$ to $i\hbar/(1+\beta)$ while the x and y commutators are unaffected. The kinetic energy term in the Schrödinger equation, $-\hbar^2\nabla^2/2m$, is therefore perturbed by the amount

$$V^K = \left(\frac{1}{(1+\beta)^2} - 1\right)\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial z^2} = \frac{2\beta+\beta^2}{(1+\beta)^2}\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}. \tag{21}$$

The second derivative, expressed in polar coordinates r, $\xi = \cos\theta$, and ϕ is

$$\begin{aligned}\frac{\partial^2}{\partial z^2} &= \xi^2 \frac{\partial^2}{\partial r^2} + \frac{2\xi(1-\xi^2)}{r}\frac{\partial}{\partial r}\frac{\partial}{\partial \xi} + \frac{(1-\xi^2)^2}{r^2}\frac{\partial^2}{\partial \xi^2} - \\ &\quad - \frac{3\xi(1-\xi^2)}{r^2}\frac{\partial}{\partial \xi} + \frac{1-\xi^2}{r}\frac{\partial}{\partial r} \end{aligned} \tag{22}$$

Using these results, the matrix elements are found to be

$$\begin{aligned} V^K_{21m,21m} &= -\frac{41}{120}\frac{2\beta+\beta^2}{(1+\beta)^2}\frac{Ze^2}{a}, \\ V^K_{210,210} &= -\frac{7}{120}\frac{2\beta+\beta^2}{(1+\beta)^2}\frac{Ze^2}{a}, \\ V^K_{200,200} &= -\frac{1}{3}\frac{2\beta+\beta^2}{(1+\beta)^2}\frac{Ze^2}{a}, \\ V^K_{100,100} &= -\frac{1}{3}\frac{2\beta+\beta^2}{(1+\beta)^2}\frac{Ze^2}{a}. \end{aligned} \tag{23}$$

The other matrix elements vanish.

These enable the calculation of the atomic frequencies radiated at a point where β is the value of our Schwartzchild parameter. We must multiply by the gravitational red shift $1/\sqrt{1+\beta}$ if the radiation is observed at infinity. The results, both with and without the effect of modifying the commutation rules and with and without the gravitational red shift, are shown in the figure.

In order to assess these results in terms of the observability of the effect of modifying the commutation rules, we must have a measure of the broadening expected.

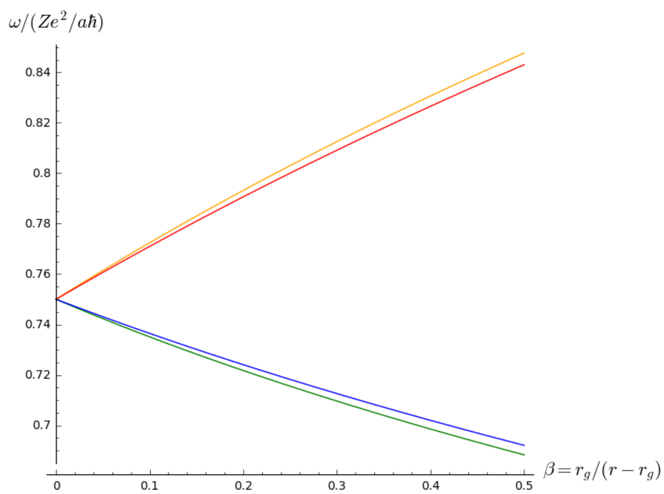

Figure 1: Frequency of the $2p \to 1s$ transition in units of $Ze^2/\hbar a$ as a function of $\beta = r_g/(r - r_g)$. The effects of gravitational distortion of the Coulomb potential, the gravitational red shift and the modification of the commutation rules are included in the green curve. The blue curve omits the effect of modifying the commutation rules. The red and orange curves show the same without the gravitational red shift.