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INFLUENCE OF THE ELECTRON'S ANOMALOUS MAGNETIC DIPOLE MOMENT ON HIGH-ATOMIC NUMBER ATOMS

by

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ABSTRACT

Super-heavy atoms ($Z > 100$) are usually studied in the context of the so-called " Quantum Electrodynamics of Strong Fields ". In this theory the problem of the singularity in the electron energy whenever $Z > 137$ is overcome. This is done by considering the finite size of the nucleus and leads to interesting phenomena, such as the spontaneous production of positrons. Here, we show that, taking into account the contribution from the Anomalous Magnetic Dipole Moment of the electron (by means of an effective theory), within a point nucleus model, is a sufficient condition to obtain regular wave functions and physically acceptable energy values for $Z > 137$.

Key-words: Superheavy atoms; Strong electromagnetic fields.

1. INTRODUCTION

In the last fifteen years a great deal of attention has been given to the problem of atoms with very high atomic numbers, $Z > 137$. At sufficiently small distances the radial solutions of the Dirac equation for an electron in the field of a point charge $Z|e|$ behave as $r^{\pm\gamma}$, where

$$\gamma = \left[(j + 1/2)^2 - (Z\alpha)^2 \right]^{1/2} \tag{1.1}$$

and $\alpha = e^2 = 1/137$ is the fine structure constant. Now if $Z\alpha > j + 1/2$, γ becomes a pure imaginary number and the solution oscilates infinitely many times as $r \to 0$ and no boundary condition can be imposed at $r = 0$.

This difficulty disappears when one acknowledges the finite size of the nucleus. This provides a cut-off for the attractive Coulomb field and meaningful solutions which behave regularly at the origin can be found for any Z. The theory presents some interesting novel features such as the decay of the neutral vacuum into a charged vaccum by spontaneous emission of positrons [1,2,3,4]. These predictions have been observed in U-Cm and U-U- collisions [5].

In this paper we present an alternative way to regularize the wave-functions at $r = 0$. As Grandy [6] pointed out, this can be done if one takes into account the anomalous magnetic dipole moment (AMDM) of the electron through the Pauli effective Hamiltonian (see below). We then show that well behaved functions can be obtained, even in the case of a point nucleus. The system behaves pretty much as the finite nucleus model and all the interesting new phenomena which appear therein are also present in this new focalization.

2. ANOMALOUSLY MAGNETIZED ELECTRON IN THE FIELD OF A POINT NUCLEUS

The AMDM of the electron can be taken into account by adding to Dirac's equation a phenomenological new term due to Pauli. The thus modified equation is [7]

$$\left[\gamma^{\mu}(p_{\mu} - eA_{\mu}) - m \right] \psi = (ae/2m)(1/2)\sigma^{\mu\nu} F_{\mu\nu} \psi \qquad (2.1)$$

Here, $a = (g-2)/2$ is the ratio between the AMDM and the Bohr magneton. We shall take a static point nucleus with charge $Z[e]$, so that the potential 4-vector is given by

$$A^{\mu} = (Z|e|/r, \vec{0}) \qquad (2.2)$$

Then (2.1) can be put in the form

$$i \frac{\partial\psi}{\partial t} = H\psi \qquad (2.3)$$

with

$$H = \gamma^{o} \vec{\gamma} \cdot \vec{p} + m\gamma^{o} - \frac{Z\alpha}{r} - (iaZ\alpha/2mr^{2})\vec{\gamma}\cdot\hat{r} \qquad (2.4)$$

where $\hat{r} = \vec{r}/|\vec{r}|$ is the unit radial vector and γ^{o} and $\vec{\gamma}$ are the Dirac matrices. Now, since the anomalous term $(-iaZ\ /2mr^{2})(\vec{\gamma}\cdot\hat{r})$ comutes with J^{2}, J_{z} and with the parity operator, the wave function can be put in the form

$$\psi = \frac{1}{r} \begin{pmatrix} U_{1}(r)\ \Omega^{m}_{k}\ (\hat{r}) \\ \\ i\ U_{2}\ (r)\ \Omega^{m}{}_{k}(\hat{r}) \end{pmatrix} \qquad (2.5)$$

where Ω^{m}_{k} is a spherical Pauli spinor and $-k = \pm\ (j + 1/2)$ is the eigenvalue of the spin-orbit operator $\gamma^{o}(\vec{\Sigma}.\vec{L}+1)$. The radial functions U_{1} and U_{2} satisfy the coupled equations [8] .

$$\frac{dU_{1}}{dr} + \left(\frac{k}{r} - \frac{aZ\alpha}{2mr^{2}} \right) U_{1} = \left(m + E + \frac{Z\alpha}{r}\right) U_{2}$$

$$\frac{dU_{2}}{dr} - \left(\frac{k}{r} - \frac{aZ\alpha}{2mr^{2}} \right) U_{2} = \left(m - E - \frac{Z\alpha}{r}\right) U_{1} \qquad (2.6)$$

3. THE WAVE-FUNCTION FOR $r \ll 1/m$

The set of equations (2.6) has two essential singularities at $r = 0$ and $r = \infty$ and is very difficult to solve exactly. Nevertheless, its behaviour near the origin can be found by neglecting the terms $m + E$ and $m - E$ which, in this region, are small compared to $Z\alpha/r$. By introducing $x = mr$, we then have the truncated equations

$$\frac{dU_1}{dx} + \left(\frac{k}{x} - \frac{aZ\alpha}{2x^2}\right)U_1 = \frac{Z\alpha}{x}\, U_2$$

$$\frac{dU_2}{dx} - \left(\frac{k}{x} - \frac{aZ\alpha}{2x^2}\right)U_2 = -\frac{Z\alpha}{x}\, U_1 \tag{3.1}$$

which are freed of the essential singularity at $x = \infty$. The decoupling of these equations leads to

$$\frac{d^2U_1}{dx^2} + \frac{1}{x}\frac{dU_1}{dx} + \left[\frac{(Z\alpha)^2-k^2}{x^2} + \frac{(2k+1)aZ\alpha}{2x^3} - \frac{(aZ\alpha)^2}{4x^4}\right]U_1 = 0$$

$$\frac{d^2U_2}{dx^2} + \frac{1}{x}\frac{dU_2}{dx} + \left[\frac{(Z\alpha)^2-k^2}{x^2} + \frac{(2k-1)aZ\alpha}{2x^3} - \frac{(aZ\alpha)^2}{4x^4}\right]U_2 = 0 \tag{3.2}$$

Because $x = \infty$ is a regular point we introduce a new variable

$$y = aZ\alpha/x \tag{3.3}$$

and new functions

$$v_{1,2} = y^{1/2}\, U_{1,2} \tag{3.4}$$

in terms of which, (3.2) becomes

$$\frac{d^2v_1}{dy^2} + \left[-\frac{1}{4} + \frac{k+1/2}{y} + \frac{(Z\alpha)^2-k^2+1/4}{y^2}\right]v_1 = 0$$

$$\frac{d^2v_2}{dy^2} + \left[-\frac{1}{4} + \frac{k-1/2}{y} + \frac{(Z\alpha)^2-k^2+1/4}{y^2}\right]v_2 = 0 \qquad (3.5)$$

The solutions of (3.5) which satisfy the boundary conditions $U_1(x)$, $U_2(x) \to 0$ as $x \to 0$ $(y \to \infty)$ are Whittaker functions of second kind [9]

$$v_1 = A_1\, W_{k+1/2,\gamma}(y)$$

$$v_2 = A_2\, W_{k-1/2,\gamma}(y) \qquad (3.6)$$

where γ is given in (1.1). To determine the relation between A_1 and A_2 we substitute (3.6) back in (3.1) thus obtaining

$$A_2/A_1 = -Z\alpha \qquad (3.7)$$

So that, considering (3.3) and (3.4), we have

$$U_1 = A(x/aZ\alpha)^{1/2}\, W_{k+1/2,\gamma}(aZ\alpha/x)$$

$$U_2 = -AZ\alpha(x/aZ\alpha)^{1/2}\, W_{k-1/2,\gamma}(aZ\alpha/x) \qquad (3.8)$$

where A is a normalizing constant. The Whittaker function remains real as $Z\alpha$ surpasses $j + 1/2$ and γ becomes imaginary [3,4] so no problem appears in the boundary condition at $r = 0$. From the asymptotic behaviour of the Whittaker function

$$W_{m,\gamma}(y) \sim y^m \exp(-y/2) \text{ as } y \to \infty \qquad (3.9)$$

we obtain the behaviour of the wave function near r = 0.

$$U_1(x) \simeq A(aZ\alpha/x)^k \exp(-aZ\alpha/2x)$$

$$\text{as } x \to 0 \qquad (3.10)$$

$$U_2(x) \simeq AZ\alpha(aZ\alpha/x)^{k-1} \exp(-aZ\alpha/2x)$$

From (3.10) we see that, as long as $a > 0$, the exponential factor dominantes and the wave function dies off as $x \to 0$. (If $a < 0$, one makes the substitution $y = -aZ\alpha/x$ instead of (3.3) and again, one gets well behaved solutions near $x = 0$ which can be obtained from (3.8) by the transformation $a \to -a$, $k + 1/2 \to -k \mp 1/2$). Note that near the origin the wave function is independent of γ'. The effect that the AMDM can render an ill-defined Dirac equation self-adjoint was noticed before by Goldhaber et al [10] in the context of the Dirac equation in the field of a magnetic monopole.

4. NUMERICAL RESULTS AND QUALITATIVE ANALISIS

In order to find the eigenvalues of energy we decoupled the set of equations (2.6) and made the transformation[8].

$$U_i = [m + (E + Z\alpha/r)\varepsilon_i]^{1/2} \chi_i(r) \qquad (4,1)$$

where $i = 1,2$; $\varepsilon_1 = +1$; $\varepsilon_2 = -1$. By defining

$$h_i(r) = 1 + (E - m\varepsilon_i)r/Z\alpha \qquad (4.2)$$

we find that the transformed functions χ_i satisfy the Schrödinger-type equation

$$- \chi_i''(r) + V_{eff}^{(i)}(r)\,\chi_i(r) = \omega^2\,\chi_i(r) \tag{4.3}$$

where

$$\omega^2 = E^2 - m^2 \tag{4.4}$$

and

$$V_{eff}^{i} = -2EZ\alpha/r + \left[k(k+\varepsilon_i) - (Z\alpha)^2 \right]/r^2 - (1+k\varepsilon_i)/r^2 h_i(r) + 3/4r^2 h_i^2(r) - (k+\varepsilon_i)\,aZ\alpha\varepsilon_i/mr^3 + aZ\alpha\varepsilon_i/2mr^3 h_i(r) + (aZ\alpha)^2/4m^2r^4 \tag{4.5}$$

Observe that the energy-dependent effective potential (4.5) has a repulsive term $(aZ\alpha)^2/4m^2r^4$ which at small distances dominates and cuts off the Coulomb attraction. This $1/r^4$ term plays here a role analogous to the cut-off in the potencial of the finite nucleus model.

In order to solve (4.3) numerically, one first has to decide which value of a to use in the effective potential (4.5). If we take the infrared limit $a = \alpha/2\pi$, then (3.10) indicates the AMDM leads to a cut-off of the wave function at distances $aZ\alpha/2mr \sim 1$ or $r \sim aZ\alpha/4\pi m < 1$ fm, corresponding to momenta of almost 1 Gev/c. However, the infrared limit of the AMDM is obtained from the form factor in the limit $|\vec{p}| \ll m \sim 0{,}5$meV/c. It is therefore, questionable if the infrared limit can be applied. On the other hand Ritus [11] has shown that in the context of a uniform electric field ε (as well as magnetic) the AMDM depends on the field and on the momentum component transverse to the field. For null transverse momentum and very strong field ($e\varepsilon/m^2 \gg 1$) the AMDM is twice that of the infrared limit, that is $a = \alpha/\pi$. In the case considered here, the electron gets so close to the nucleus that the above condition on the field is certainly satisfied. So, it is reasonable to guess that, at least for S waves (which have no transverse momentum to the field) the same limit may be applied.

Equation (4.3) was solved numerically in both limits. The eigen values thus obtained are plotted in fig. 1 (Together with the finite nucleus model results [12] for comparison). The numerical method we used requires that $(\partial V_{eff}/\partial E)-2E$ has the same sign for all r. This condition is satisfied only for i = 1, k < 0. We were thus unable to verify if the fast diving of the $2P_{1/2}$ state (k = +1) observed for extended nuclei also happens in the case studied here. The shape of the curves in fig. 1 can be qualitatively understood as follows: suppose we know the eigenvalues of the Hamiltonian (2.4) at a given Z value

$$H(Z)\psi_{nk} = E_{nk}(Z)\psi_{nk} \qquad (4.6)$$

and let us examine what happens when the atomic number is increased by a small amount δZ. We have

$$H(Z + \delta Z) = H(Z) + \delta Z\; U \qquad (4.7)$$

where

$$U = -\alpha/x - (ia\alpha/2x^2)\vec{\gamma}.\hat{r}$$

The variation in energy can be found by perturbation theory. In first order we have

$$\delta E = \delta Z <\psi|U|\psi> \qquad (4.8)$$

then, using (2.5) we get

$$dE/dZ = -\alpha \int dx(U_1^2+U_2^2)/x - a\alpha \int dx\; U_1U_2/x^2 \qquad (4.9)$$

In the case a = 0, (4.9) looses its meaning for $Z\alpha > 1$, because the integrals diverge. For a > 0, however, the exponential factors in (3.10) ensure the convergence for any Z, as long as $|E| < m$. The first term in (4.9) is negative. The second is positive, at least in the ground state, since, in this case, U_1 and U_2 have opposite signs, as one can see from (3.10) and from the fact that the ground state wave function has no nodes. Nevertheless, since a is so small ($\sim 10^{-3}$), the second term contributes little and $dE/dZ < 0$.

Furthermore, one can see that d^2E/dZ^2 is also negative. The most important contribution to the integrals in (4.9) comes from the region around the maxima of U_1 and U_2. As Z increases, these maxima move towards $x = 0$ (the electron gets closer to the point nucleus), therefore, increasing the contribution of the 1/x factor in the first integral. So, we can presume that the derivative dE/dZ increases in absolute value as Z increases. So, E is a decreasing function of Z with negative curvature.

It is then clear, that, just as in the finite nucleus model, as the atomic number increases, a value, called critical Z, will be attained, for which $E = -m$. Evidently this number will depend on the quantum numbers n and k of (4.6). The largest integer for which $E > -m$ was found to be $Z = 159$ (198) for 1S(2S) waves and $a = \alpha/2\pi$. For $a = \alpha/\pi$ these values change to 164 and 209, respectively. As Z increases further, the previously discrete state will become a member of the negative continuum as (4.9) indicates. These over-critical states can be singled out from other members of the continuum by the shape of their wave-functions. The wave function of the continuum states are pratically zero within the atom but, as the energy approaches the "dived in" state energy, a highly pronounced peak appears near $r = 0$, which is characteristic of ressonant states. This situation is illustrated in fig. 2, for $a = \alpha/2\pi$. To obtain this "dived in" ressonant 1S state we extrapolated the E(Z) function obtained for the undercritical 1S state to $Z = 160$, the first over critical atomic number. Next we put this energy value back in (2.6) and solved the resulting set of equations by an initial value method. The initial values for U_1 and U_2 were obtained from (3.8) at $x = mr = 10^{-5}$. Then by a careful search around this energy value we looked for the ressonant behaviour described above and found an extremely narrow peak at $E = -1,074969485$ electron masses. Fig. 1 also shows the wave function for a non ressonant energy value.

5. CONCLUSION AND ACKNOWLEDGMENTS

In conclusion, we have seen that the AMDM does regularize the wave functions at $r = 0$, even for point nuclei.

As for the value of the critical atomic number, this will depend on the anomalous magnetization the electron attains at strong fields. We also suggest that the combined effects of boths the finite size of the nucleus and the AMDM should be explored before a conclusion as to the precise value of the critical charge can be reached.

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FIGURE CAPTIONS

Fig. 1. - ExZ curves

- - - - finite nucleus[12]

______ point nucleus, AMDM model, $a = \alpha/2\pi$

-.-.-.- point nucleus, AMDM model, $a = \alpha/\pi$

(for 2 $P_{3/2}$ waves, the three curves coincide).

Fig. 2 - Super critical $U_1^2 + U_2^2$ function in the point nucleus + AMDM model, with $a = \alpha/2\pi$.

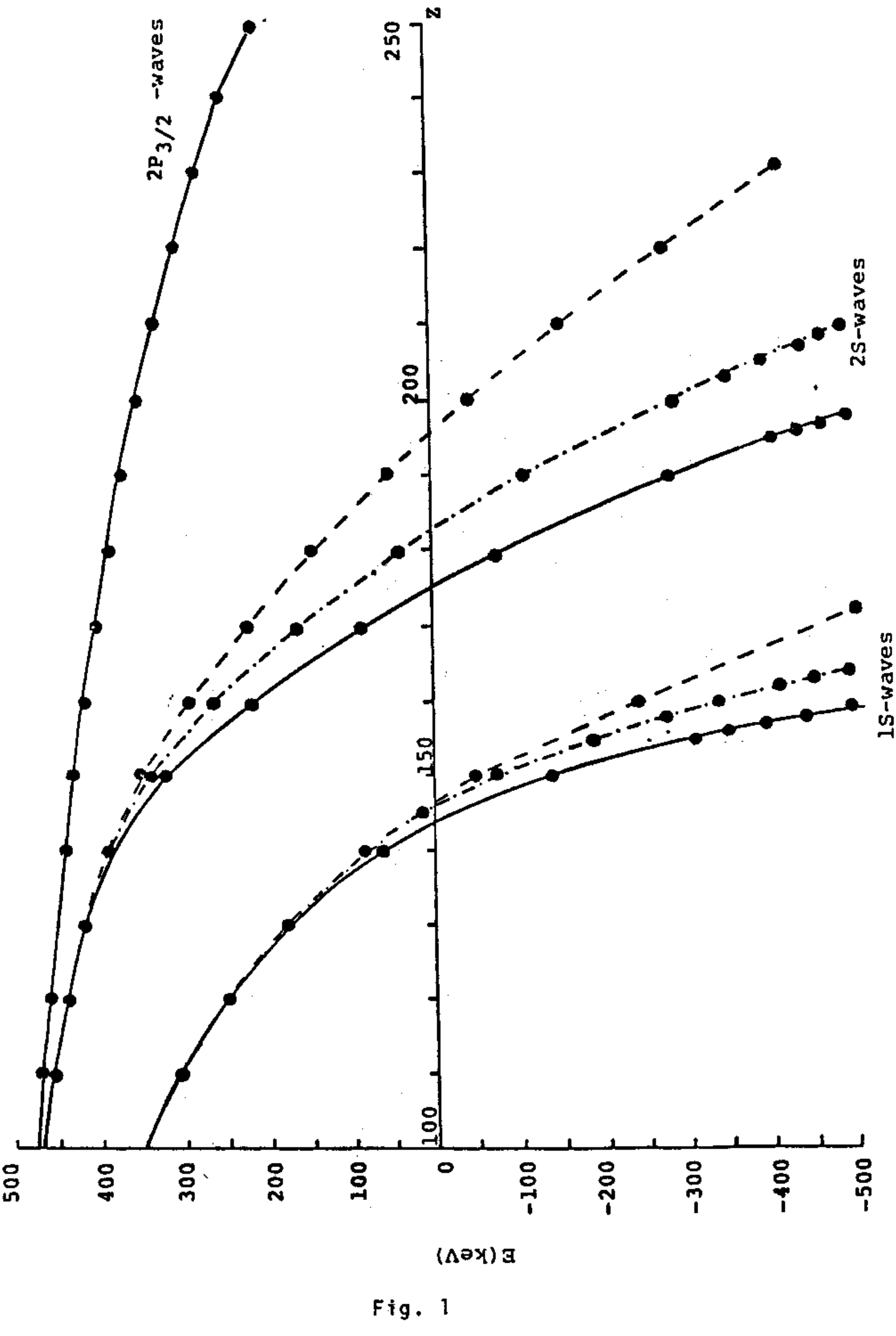
2P3/2 -waves
2S-waves
1S-waves
Z
250
200
150
100
500
400
300
200
100
0
-100
-200
-300
-400
-500
E(keV)

Fig. 1

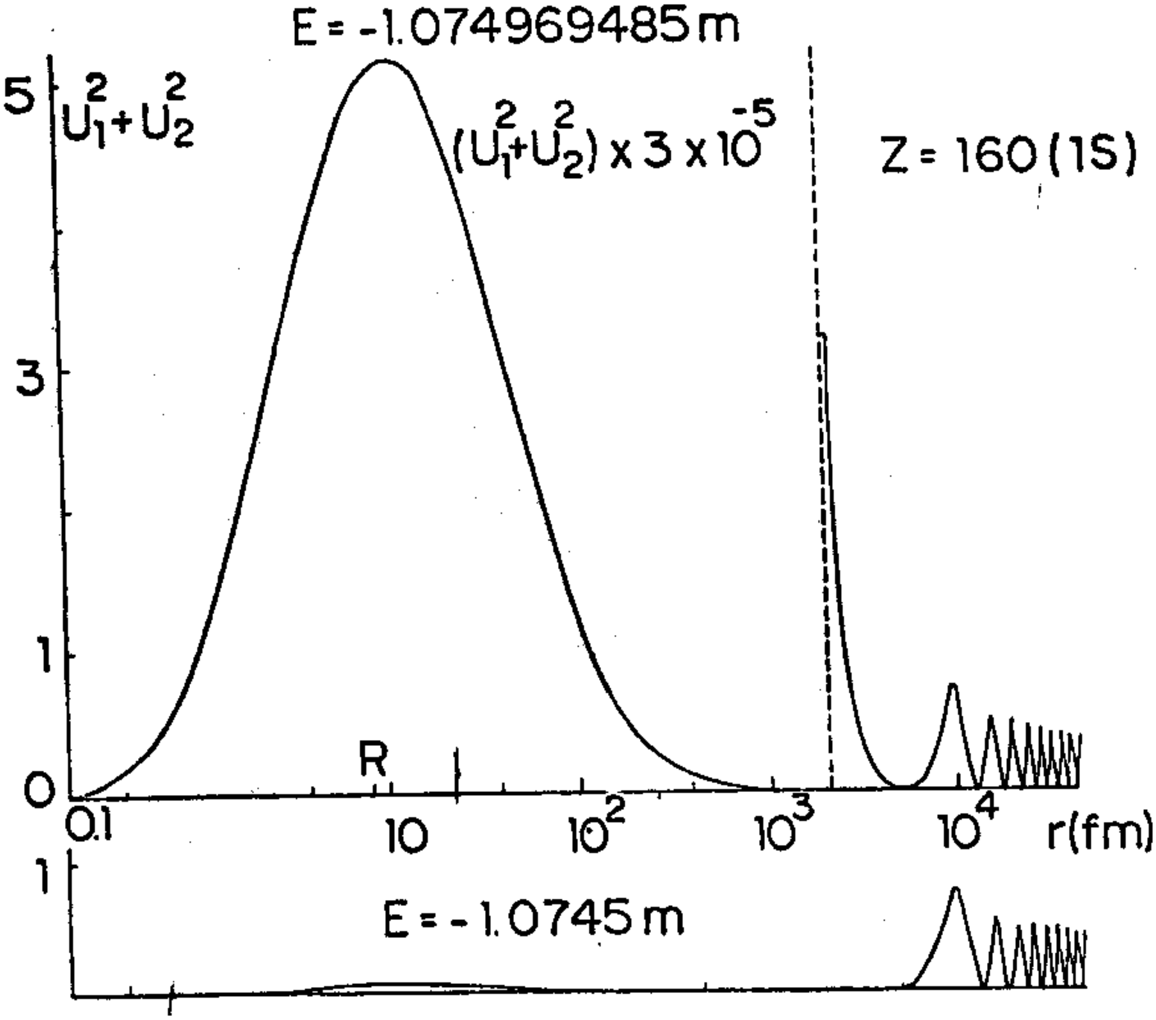
E = -1.074969485 m
5
$U_1^2+U_2^2$
$(U_1^2+U_2^2) \times 3 \times 10^{-5}$
Z = 160 (1S)
3
1
R
0
0.1
10
10^2
10^3
10^4
r(fm)
1
E = -1.0745 m

Fig. 2

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