# ENERGY LEVELS AND APPROXIMATE WAVE FUNCTIONS OF MESIC ATOMS

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Submitted to JETP editor January 20, 1959

J. Exptl. Theoret. Phys. (U.S.S.R.) 36, 1806-1817 (June, 1959)

A calculation of the energies of the 1S, 2S, 3S, 2P, and 3P levels of mesic atoms is made in nonrelativistic approximation for a constant distribution of the charge density of the nucleus inside a sphere of radius  $R_0$ . By numerical solution of the Schrödinger equation formulas are found for the dependence of the quantum defect  $\Delta n$  on the quantity  $t = R_0 Z/a_{\mu}$  ( $a_{\mu}$  is the Bohr radius of the meson orbit). Approximate wave functions are given for the corresponding states. It is shown how to use these wave functions in perturbation theory to find relativistic corrections and level shifts arising from a change of the shape of the charge distribution of the nucleus.

### 1. INTRODUCTION

THERE has recently been great interest in processes associated with the distribution of the positive charge inside the nucleus. One of the means for studying this distribution is  $\mu$ -mesic atoms.<sup>1-3</sup> For the interpretation of the experimental data one must be able to calculate the positions of the energy levels of the meson in a mesic atom for various distributions of the charge of the nucleus, and also to calculate a number of other effects that affect the positions of the levels.

The problem of mesic atoms differs considerably from that of ordinary electronic atoms. First of all, a mesic atom is hydrogenlike. The probability of capture of two or more mesons by a single atom is very small, and the electrons of the atom, being much farther from the nucleus, have practically no effect on the motion of the meson.\* On the other hand the size and shape of the nucleus have important effects on the motion of the meson. The Bohr radius of the meson orbit,  $a_{\mu} = \hbar/me^2$  (m is the reduced mass of the meson) is 200 to 300 times smaller than the electronic Bohr radius, since the mass of the meson is this many times larger than that of the electron. Calculations show that in heavy  $\mu$ -mesic atoms the meson spends

more than half of the time inside the nucleus.<sup>1</sup> In first approximation the nucleus can be regarded as a sphere uniformly charged with positive electricity. Therefore a heavy mesic atom is to a high degree reminiscent of the Thomson model of the atom with an oscillator potential inside the nucleus. It still turns out, however, that though for mesic atoms with Z < 10 the Rutherford model with a point nucleus is a good approximation (the correction to the energy levels caused by the finite volume of the nucleus is not more than 1 percent), even for the heaviest mesic atoms the Thomson model (with an oscillator potential of infinite extent),<sup>4,5</sup> though it is a better approximation than the Rutherford model, cannot be taken as a zeroth approximation if one wants to get really good results (cf. Fig. 1).

Thus the basic difficulties in the calculation of the energy levels of mesic atoms (for  $\mu$  or  $\pi$  mesons with Z > 10) lie in the fact that there does not exist an exact solution of the wave equation (even for the simplest types of distribution of the charge of the nucleus) that can be taken as the zeroth approximation. It must be pointed out that all other factors affecting the positions of the levels (small changes of the charge distribution inside the nucleus, magnetic and electric moments of the nucleus, vacuum polarization, polarization of the nucleus by the meson, and so on) $^{1-4,6,7}$  give corrections to the levels that are of the order of 1 to 2 percent, and consequently can be calculated by first-order perturbation theory, at least in the present situation as to experimental accuracy. The relativistic corrections are also rather small.<sup>4,8</sup> Because of the smearing out of the charge over the volume of the nucleus these cor-

<sup>\*</sup>This is true, of course, if we are interested in the motion of the meson and its spectrum. On the other hand, the presence of the meson in a mesic atom has considerable effect on the motion of the electrons. Because of the screening of the nucleus by the meson the effective charge producing the field in which the electrons move is reduced practically by unity, and from the point of view of chemical and optical properties the atom must be shifted one place to the left in the periodic table.



FIG. 1. Dependence on the parameter t of the shift of the 1S level owing to the effect of the volume of the nucleus, as found by various methods: 1) first-order perturbation theory with Kepler wave functions: a) complete result, b) first term of expansion in powers of t ( $\Delta E/E_0 \approx 0.8t^2$ ); 2) first-order perturbation theory with oscillator wave functions;<sup>5</sup> 3) variation method;<sup>12</sup> 4) expansion of the right member of Eq. (4) in powers of  $\Delta n$  (including term in ( $\Delta n$ )<sup>2</sup>); 5) asymptotic representation (not distinguishable on this scale). For cases 4 and 5 the left member of Eq. (4) was calculated from Eq. (14). The scale of Z on the axis of abscissas is given for  $\mu$ -mesic atoms ( $R_0 = 1.2A^{4}_{4} \times 10^{-13}$  cm).

rections for heavy nuclei are somewhat smaller than the corresponding quantities as found from the formulas for point nuclei, i.e., from the usual fine-structure formulas.

With electronic computers available one can of course find to any degree of accuracy the solution of any relativistic equation with the potential given by a prescribed distribution of the charge of the nucleus, as has been done, for example, in the paper of Ford and Hill.<sup>7</sup> But the programming for an electronic computer is in itself rather laborious, and the presence of many parameters does not allow the possibility of foreseeing all the choices for which the need may arise. In many investigations there is often no need to know the result with high precision, but one does need to be able to find rather quickly an approximate value of a quantity and to know how it will change with changes of a number of parameters. Therefore it is desirable to have a sufficiently simple approximate solution that can be taken as a zeroth approximation and gives the possibility of calculating the effects of

various factors on the position of the levels of mesic atoms by the universally familiar methods of perturbation theory.

Formulas are obtained in this paper that permit us to find the first five energy levels of mesic atoms in nonrelativistic approximation for a constant distribution of charge density inside the nucleus. Approximate wave functions are given, and also examples of the calculation with these wave functions of several corrections to the levels by means of perturbation theory.

# 2. DETERMINATION OF THE SOLUTION OF THE WAVE EQUATION

For a uniform distribution of the charge of the nucleus inside a sphere of radius  $R_0$  the charge density

$$\rho(r) = 3eZ / 4\pi R_0^3, \qquad 0 \leqslant r \leqslant R_0,$$

$$\rho(r) = 0, \qquad R_0 < r \leqslant \infty \qquad (1)$$

corresponds to a Thomson (oscillator) potential inside the nucleus and a Coulomb potential outside:

$$\varphi(r) = (eZ/R_0) [^3/_2 - \frac{1}{2} (r/R_0)^2], \quad 0 \le r \le R_0,$$
  

$$\varphi(r) = eZ/r, \quad R_0 \le r \le \infty. \quad (2)$$

The basis taken for the determination of the approximate energy eigenvalues and approximate wave functions was the solution of the nonrelativistic Schrödinger equation with the potential (2). After separation of the variables one gets for the radial part R(r) of the wave function the equation

$$\frac{d^{2}R}{dr^{2}} + \frac{2dR}{rdr} + \left(\frac{2m}{\hbar^{2}}E + \frac{2me}{\hbar^{2}}\varphi(r) - \frac{l(l+1)}{r^{2}}\right)R = 0.$$
 (3)

The reasons for the choice of this equation are, firstly, that it is the same for mesons of any spin; the relativistic and spin corrections can be found by perturbation theory, if the nonrelativistic solution is known. Secondly, in this case the solution is a function of only one parameter,  $t = R_0 Z/a_{\mu}$ . Owing to the linear dependence of t on the mass of the meson, the radius of the nucleus, and the atomic number, it is very easy to find the change of the energy of a level with change of any of these three parameters.

The method of matching was used to find the energy eigenvalues. In this method one requires continuity of the wave function and its first derivative at the edge of the nucleus, or, what is equivalent but more convenient for the unnormalized functions, continuity of the logarithmic derivative:

$$\frac{d}{dr}(\ln R_i)_{r=R_0} = \frac{d}{dr}(\ln R_e)_{r=R_0}.$$
(4)

Here  $R_i(r)$  and  $R_e(r)$  are solutions of Eq. (3)

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respectively inside and outside the nucleus. On  $R_i$  we impose the requirement of finiteness at the origin, and Re must vanish at infinity. The equation (4) is a transcendental equation for the energy E, which occurs as a parameter in  $R_i$ and R<sub>e</sub>. The energy eigenvalues can be found by numerical solution of this equation.

Let us introduce

$$x = r/R_0, \quad x^{-t}R(x) = y(x), \quad t = R_0 Z/a_{\mu},$$

$$E_0 = -me^4 Z^2/2\hbar^2$$
,  $\varepsilon = E/E_0$ ,  $\gamma = \varepsilon^{-1/2}$ . (5)  
Here  $E_0$  is the energy of the ground state of the  
meson for a point nucleus. The quantity  $\gamma$  has  
the meaning of an effective quantum number and  
can be represented in the form

$$\gamma = n + \Delta n, \tag{6}$$

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where n is an integer that defines the number of the shell in which the meson is (principal quantum number), and  $\Delta n$  is the addition caused by the finiteness of the nuclear volume (quantum defect).\* Using the notation of (5) we get from Eq. (2) an expression for the potential energy of the meson in the field of the nucleus  $[U_0 = -e\varphi(\mathbf{r})]$ :

$$U_0 = (E_0/t)(3-x^2), \qquad 0 \leqslant x \leqslant 1,$$
$$U_0 = 2E_0/tx, \qquad 1 \leqslant x \leqslant \infty$$
(7)

and from Eq. (3) we get two equations for the regions inside and outside the nucleus, respectively:

$$\frac{d^2y_i}{dx^2} + \frac{2(l+1)}{x}\frac{dy_i}{dx} - [t(\varepsilon t - 3) + tx^2]y_i = 0,$$
  
$$0 \leqslant x \leqslant 1,$$
 (8a)

$$\frac{d^2y_e}{dx^2} + \frac{2(l+1)}{x}\frac{dy_e}{dx} - \left(\frac{t^2}{\gamma^2} - \frac{2t}{x}\right)y_e = 0,$$

$$1 \leqslant x \leqslant \infty.$$
(8b)

a) Solution of the wave equation inside the nucleus. We can represent the solution of Eq. (8a) in the form of a power series

$$y_{l}(x) = \sum_{k=0}^{\infty} a_{k} x^{k}, \qquad (9)$$

with its coefficients connected by the recurrence relation

$$a_{k} = [t(\varepsilon t - 3) a_{k-2} + t a_{k-4}] / (2l + k + 1) k.$$
 (10)

The series contains only the even powers of x; for simplicity we take the arbitrary coefficient  $a_0$ to be unity.

For the quantity  $z = d(\ln y_i)/dx$  we can get

from Eq. (8a) a first-order differential equation of the Riccati type

$$\frac{dz}{dx} + z^2 + \frac{2(l+1)}{x}z = t(tz - 3) + tx^2.$$
(11)

The solution of this equation that corresponds to the solution of Eq. (8a) given by Eq. (9) is a power series containing only odd powers of x:

$$z = \sum_{k=1}^{\infty} b_k x^k.$$
 (12)

The first two coefficients in this series are

$$b_{1} = t(\varepsilon t - 3) / [2(l+1) + 1],$$
  
$$b_{3} = (t - b_{1}^{2}) / [2(l+1) + 3],$$

and subsequent ones can be found by means of the recurrence formula

$$b_{k} = - [2(l+1)+k]^{-1} \sum_{j=1}^{k-2} b_{j}b_{k-1-j}$$
 (k>3). (13)

If the coefficients  $b_k$  have been found, the left member of Eq. (4) can be put in the form

$$\frac{d}{dx}(\ln R_i)_{x=1} = l + \frac{d}{dx}(\ln y_i)_{x=1} = l + \sum_{k=1}^{\infty} b_k.$$
 (14)

b) Solution of the wave equation outside the nucleus. The solution of Eq. (8b) that vanishes at infinity can be expressed in terms of the Whittaker function (cf. e.g., reference 9):\*

$$y_e(x) = c_1 x^{-(l+1)} W_{\gamma, l+1/2}(2tx / \gamma).$$
(15)

For large values of x we can also represent the solution (15) by the asymptotic expansion (cf. reference 10, Eq. 7.327):

$$y_{e}(x) \approx c_{2}x^{\gamma-l-1}e^{-tx/\gamma}\left[1 + (l+\gamma)(l+1-\gamma)\frac{1}{1!}\left(\frac{\gamma}{2tx}\right) + (l+\gamma)(l-1+\gamma)\times(l+1-\gamma)(l+2-\gamma)\frac{1}{2!}\left(\frac{\gamma}{2tx}\right)^{2} + (l+\gamma)(l-1+\gamma)(l-2+\gamma)(l+1-\gamma) \times (l+2-\gamma)(l+3-\gamma)\frac{1}{3!}\left(\frac{\gamma}{2tx}\right)^{3} + \dots\right].$$
 (16)

The coefficients  $c_1$  and  $c_2$  are determined by matching the expressions (9), (15), and (16).

Using the recurrence relation for the derivative of the Whittaker function (cf. reference 10, Eq. 7.334,3), we find the right member of Eq. (4): d

$$\frac{w}{dx}(\ln R_{e}(x))_{x=1} = (\gamma - l - 1) (\gamma + l)$$

$$\frac{W_{\gamma-1, l+1/2}(2t/\gamma)}{W_{\gamma, l+1/2}(2t/\gamma)} - 1 - \frac{t}{\gamma} + \gamma.$$
(17)

\*The Whittaker function with half-integral second index has a logarithmic singularity at the origin. For its series representation see, for example, reference 10, Eq. 7.338.

<sup>\*</sup>Unlike the quantum defect used to describe the spectral series of the alkali elements,  $\Delta n$  is a positive quantity in the case of mesic atoms.

TABLE I

	1S 2S		35	2 <i>P</i>	3P	
$ \begin{array}{c} A_{0} \\ A_{1} \\ A_{2} \\ A_{3} \\ A_{4} \\ A_{5} \\ B_{1} \\ B_{2} \\ B_{3} \\ B_{4} \\ C_{0} \\ C_{2} \end{array} $	$\begin{array}{c} -0.032885\\ 0.165892\\ 0.013883\\ -0.008312\\ 0.001082\\ -\\ -\\ 5.0446\\ 0.9826\\ -0.5560\\ 2.9875\\ 0.032885\\ -\\ -\\ \end{array}$	$\begin{array}{c} -0.038028\\ 0.179527\\ 0.000123\\ -0.004548\\ 0.000635\\\\\\ 4.7209\\ 0.6281\\0.4890\\ 1.9286\\ 0.038028\\\\ -\end{array}$	$\begin{array}{c} -0.038028\\ 0.179527\\ 0.000123\\ -0.005011\\ 0.000715\\\\ 4.7209\\ 0.6281\\ -0.4890\\ 1.9286\\ 0.038028\\\end{array}$	$\begin{array}{c}$	$\begin{array}{c}$	

The expression (17) can also be written in terms of the asymptotic expansion of the Whittaker function.\*

#### 3. RESULTS OF THE NUMERICAL SOLUTION

To get the dependence of the meson energy levels on the parameter t, and the approximate wave functions, Eqs. (4) and (8a), (8b) were solved numerically for the levels † 1S, 2S, 2P, 3S, and 3P for a number of values of t in the interval  $0 \le t \le 2.75$ . This range of values provides for the computation of the energy levels of all  $\mu$ mesic and  $\pi$ -mesic atoms for  $Z \le 70$  and of K-mesic atoms for  $Z \le 20$ .

a) Determination of the energy levels. To facilitate the numerical computations preliminary values of  $\epsilon$  were found by various approximate methods. For the 1S level the results of the calculations by the approximate methods are shown in Fig. 1. The final results were obtained by the use of Eqs. (14) and (17). For the 2S and 3S levels for t > 1.5 the series (14) converges slowly, but its convergence can be considerably improved by the choice of a suitable geometrical progression.

It was found convenient to represent not the value of  $\epsilon$ , but the quantum defect  $\Delta n$  as a function of the parameter t. For the range of t indicated above, the interpolation formula

$$\Delta n = A_0 + A_1 t + A_2 t^2 + A_3 t^3 + A_4 t^4 + A_5 t^5 + (C_0 + C_2 t^2) \exp(-B_1 t - B_2 t^2 - B_3 t^3 - B_4 t^4)$$
(18)

was chosen on the basis of the individual values of  $\Delta n$  found by numerical solution (for t > 1 the

term containing the exponential can be neglected). The coefficients in the formula (18) for the various levels are shown in Table I. According to Eqs. (5) and (6) the quantity  $\epsilon$  can be calculated by the formula

$$\varepsilon = \gamma^{-2} = (n + \Delta n)^{-2}. \tag{19}$$

Use of the formulas (18) and (19) gives the value of  $\epsilon$  correct to at least four significant figures.

b) The numerical wave functions. To find  $y_i(x)$  for  $0 \le x \le 1$  we used Eqs. (9) and (10). Since computations by Eq. (15) are rather laborious, the determination of  $y_e(x)$  for  $x \ge 1$  was made by numerical integration of Eq. (8b) by the Runge-Kutta method with the initial conditions

$$y_e(1) = \sum_{k=0}^{\infty} a_k, \quad y_{e'}(1) = \sum_{k=2}^{\infty} ka_k.$$

The numerical integration was broken off at values of x for which the asymptotic representation of  $y_e(x)$  was accurate enough. Beyond this the computations were made by Eq. (16). The step for the numerical integration and the value of x at which it was broken off were chosen so that the values were obtained with an accuracy of the order of 0.001 of the value y(0) = 1. For the unnormalized wave functions so obtained the normalization constants C were found from the condition

$$C^{2}\int_{0}^{\infty} x^{2l+2} y^{2}(x) \, dx = 1 \tag{20}$$

The integral (20) was computed by Simpson's rule. Figure 2 shows the unnormalized wave functions for t = 2.279 ( $\mu$ -mesic lead, R<sub>0</sub> = 1.2 A<sup>1/3</sup> × 10<sup>-13</sup> cm).

c) Approximate wave functions. It turned out to be possible to express the wave functions inside the nucleus  $(0 \le x \le 1)$  approximately in the forms

$$R_{n_{0}}(x) = C(1 - ax^{3/2}), \qquad (21a)$$

$$R_{n1}(x) = C(1 - ax^{3/2})x.$$
 (21b)

<sup>\*</sup>Regarding the use of the asymptotic expansion to solve the Dirac equation with effects of the volume of the nucleus included, see reference 11.

<sup>&</sup>lt;sup>†</sup>For the higher levels the calculation of the energy can be made by perturbation theory with the wave functions of the Kepler problem as zeroth approximations (cf., e. g., references 2 and 7).



for S and P states respectively. The parameter a is so chosen that at x = 1 the approximate wave function equals the exact value.

Outside the nucleus (for  $x \ge 1$ ) we have represented the wave functions for the states 1S, 2P, 2S, 3P, and 3S in the respective forms

$$R_{10}(x) = Cu \exp[b(1-x)], \qquad (22a)$$

$$R_{21}(x) = Cu \, x \exp\left[b \, (1 - x)\right], \tag{22b}$$

$$R_{20}(x) = C(u - vx) \exp[b(1 - x)], \qquad (22c)$$

$$R_{31}(x) = C(u - vx) x \exp[b(1 - x)], \quad (22d)$$

$$R_{30}(x) = C(u - vx + wx^2) \exp[b(1 - x)]. \quad (22e)$$

The numerical values of the parameters u, v, w have been chosen so that, first, the approximate wave functions are continuous at the surface of the nucleus (x = 1), and second, the zeroes of the approximate wave functions for the 2S, 3P, and 3S states coincide with those of the corresponding numerically computed functions.

From the parameters found for the individual values of t, formulas were devised for the calculation of the parameters:

FIG. 2. Unnormalized functions  $x^{-1}R(x)$  for  $\mu$ mesic lead (t = 2.279): 1) solution in form of power series; 2) numerical integration; 3) asymptotic formulas;  $\rho = tx = Zr/a_{\mu}$ .

for all states 
$$\begin{cases} tb^{-1} \\ u^{-1} \end{cases}$$
  
for 2S and 3S states  $a$   
for 3P state  $(1-a)^{-1}$   
for 3S state  $v (a+u-1)^{-1}$ 

(23)

The values of the coefficients in Eq. (23) for the various parameters and states are given in Table II. The remaining parameters are determined by the formulas

$$a = 1 - u \qquad \text{for states 1S and 2P}$$

$$v = a + u - 1 \qquad \text{for states 2S and 3P}$$

$$w = 1 + v - a - u \qquad \text{for state 3S} \qquad (24)$$

The approximate wave functions thus chosen reproduce the behavior of the numerical wave functions inside the nucleus rather well (the differences of the ordinates do not exceed 2 percent). Outside the nucleus the agreement between the approximate functions and the numerical functions is poorer (especially for the 3S state). This is explained by the fact that the asymptotic behaviors of the approximate functions,  $\sim x^{n-1} \exp(-bx)$ , and the numerical functions,  $\sim x^{\gamma-1} \exp(-tx/\gamma)$ ,

State	Parameter	$D_{\mathfrak{o}}$	D <sub>1</sub>	D <sub>2</sub>	D,	
15	$u^{-1}$	1	$0,4501 \\ 0,3068$	-0.0424 0.0212	0,00580 0,00977	
2 <b>P</b>	$u^{-1}$ <i>ib</i> <sup>-1</sup>	1 2	$\substack{0.2650\\0.0015}$	0.0187 0.0388	-0.00220 -0.00333	
2 <b>S</b>	$a$ $u^{-1}$ $tb^{-1}$	$\frac{1}{2}$	$\begin{array}{c} 0.4425 \\0.0861 \\ 0.4095 \end{array}$	-0.0848 0.0382 0.0180	$0.00846 \\ -0.00314 \\ -0.01177$	
3 <b>P</b>	$(1 - a)^{-1}$ $u^{-1}$ $tb^{-1}$	1 1 3	$0,2662 \\ 0,1009 \\0.0177$	$\begin{array}{c} 0.0296 \\ -0.0183 \\ 0.0496 \end{array}$	0,00483 0,00237 0,00289	
35	$\begin{vmatrix} a \\ u^{-1} \\ v (a + u - 1)^{-1} \\ tb^{-1} \end{vmatrix}$	$\frac{1}{1}$	$\begin{array}{c} 0.4469 \\ -0.2523 \\ 0.1141 \\ 0.4464 \end{array}$	$\begin{array}{c} -0.0718 \\ 0.0813 \\ -0.0088 \\ 0.0258 \end{array}$	$\begin{array}{c} 0,00572 \\ -0,00986 \\ 0.00050 \\ -0,01305 \end{array}$	

TABLE II

0

are different. One could, of course, choose somewhat more complicated approximate wave functions, which would be much closer to the numerical functions, by taking, for example, for the function outside the nucleus an expression close to the asymptotic expression:  $x^{\gamma-1}P_{n-l-1}(x) \exp(-tx/\gamma)$  $[P_k(x)$  is a polynomial of degree k], and for the function inside the nucleus several terms of the series (9). This, however, complicates the computations for a small gain of accuracy, if the calculations are made by first-order perturbation theory.

## 4. EXAMPLES OF CALCULATIONS WITH THE APPROXIMATE WAVE FUNCTIONS

In first-order perturbation theory for a spherically symmetrical case the shift of an energy level is given by the expression

$$\Delta E = \int_{0}^{\infty} x^{2} R^{2}(x) \,\Delta U \,dx, \qquad (25)$$

where  $\Delta U = U_1 - U_0$ ;  $U_1$  is the potential energy for which one is calculating the shift of the level, and  $U_0$  is the potential energy used in the zeroth approximation, in our case that given by Eq. (7). For the calculation of the integrals (25) for the various perturbations with the approximate wave functions it is convenient to use the notations

$$F_{m} = \int_{0}^{1} (1 - ax^{3/4})^{2} x^{m} dx = \frac{1}{m+1} - \frac{4a}{2m+5} + \frac{a^{2}}{m+4}, \quad (26a)$$

$$G(\xi, m; x_{1}, x_{2}) = e^{\xi} \int_{x_{1}}^{x_{2}} x^{m} e^{-\xi x} dx$$

$$= \frac{m!}{\xi^{m+1}} \left[ e^{\xi(1-x_{1})} \sum_{k=0}^{m} \frac{(\xi x_{1})^{k}}{k!} - e^{\xi(1-x_{2})} \sum_{k=0}^{m} \frac{(\xi x_{2})^{k}}{k!} \right] \quad (26b)$$

$$H(\xi, m) = \int_{0}^{1} x^{m/2} e^{-\xi x} dx$$

$$= \frac{m (m-2) (m-4) \dots 3 \cdot 1}{(2\xi)^{(m+1)/2}} \sqrt{\frac{\pi}{\xi}} \Phi \left(\sqrt[]{2\xi}\right)$$
$$- 2e^{-\xi} \left[ \frac{1}{2\xi} + \frac{m}{(2\xi)^2} + \frac{m (m-2)}{(2\xi)^3} + \dots + \frac{m (m-2) (m-4) \dots 3}{(2\xi)^{(m+1)/2}} \right], \qquad (26c)$$

where  $\Phi(\mathbf{x}) = (2/\pi)^{1/2} \int_{0}^{\mathbf{x}} e^{-z^{2}/2} dz$  is the probability integral. Special cases of these notations are

$$G_m = G(2b, m; 1, \infty) = \frac{m!}{(2b)^{m+1}} \sum_{k=0}^m \frac{(2b)^k}{k!}, \quad G_0 = 1$$
 (26d)

$$G(\xi, m; 0, 1) = \frac{m!}{\xi^{m+1}} \left( e^{\xi} - \sum_{k=0}^{m} \frac{\xi^{k}}{k!} \right).$$
(26e)

a) The normalization coefficients. The normalization coefficient C of the approximate wave function (21a), (22a) for the 1S state can be found from the condition

$$x^{2}R^{2}(x) dx$$

$$= C^{2} \left\{ \int_{0}^{1} (1 - ax^{3/2})^{2} x^{2} dx + u^{2} e^{2b} \int_{1}^{\infty} x^{2} e^{-2bx} dx \right\} = 1. \quad (27)$$

Using Eqs. (26a and d), we get

$$C^{-2} = F_2 + u^2 G_2. \tag{28}$$

In the same way it is easy to get the normalization coefficients for the states 2S and 3S:

$$C^{-2} = F_2 + u^2 G_2 - 2uv G_3 + v^2 G_4 \qquad (2S), \qquad (29)$$

$$C^{-2} = F_2 + u^2 G_2 - 2uv G_3$$
  
+  $(v^2 + 2uw) G_4 - 2vw G_5 + w^2 G_6$  (3S). (30)  
The normalization coefficients for the 2P and 3P

The normalization coefficients for the 2P and 3P states are obtained by replacing  $F_m$ ,  $G_m$  by  $F_{m+2}$ ,  $G_{m+2}$  in Eqs. (28) and (29), respectively.

b) The relativistic corrections. For particles of spin  $\frac{1}{2}$  ( $\mu$  mesons) the relativistic corrections include (cf., e.g., reference 13): 1) the correction for the relativistic change of mass, 2) the correction for the spin-orbit interaction, and 3) a correction characteristic of the Dirac theory which has no classical analogue. For particles of spin 0 ( $\pi$  mesons) only the first correction has to be included.

1) In the case of a central field the relativistic change of mass can be taken into account in first approximation by adding to the potential energy the term

$$\Delta U' = -(2mc^2)^{-1} (U_0 - E)^2.$$
(31)

Here  $U_0$  and E are the values of the potential and total energies in zeroth approximation (E =  $\epsilon E_0$ ). Using the expression (7) for the potential energy, and also the fact that  $E_0/2mc^2 = -(\alpha Z/2)^2$ (where  $\alpha = e^2/\hbar c$  is the fine-structure constant), we get

$$\Delta U' = (\mathbf{x}Z/2t)^2 E_0 (3 - x^2 - \varepsilon t)^2, \quad 0 \le x \le 1,$$
  
$$\Delta U' = (\mathbf{x}Z/2t)^2 E_0 (2x^{-1} - \varepsilon t)^2, \quad 1 \le x \le \infty.$$
(32)

By means of the approximate wave functions (21a), (22a), the notations (26a, d), and Eq. (25) we find the correction for the relativistic change of mass

TABLE III

Mesic atom	Method of calcula- tion*	1 <i>S</i> 1/2	2P1/2	2P <sub>3/2</sub>	2S1/2	3P1/2	3P <sub>3/2</sub>	3S1/2
t = 1.1829	I	5,370	1,881	1.832	1.585			
$_{51}Sb$ t = 2.279	II I	$5,369 \\ 10.477$	1.880 4.787	1.832 4.607	1,583 3,568	2,131	2.084	1.753
$_{82}^{Pb}$ l = 2.675	II	10.477 12.112	4.780 5.924	4.604	3,561	2.127	2,081	1.747
92U	п	12.112	5.917	5,691	4.299	-		

\*I is numerical solution of the Dirac equation; II is solution with the approximate wave functions. The energy levels are given in Mev. The radius of the nucleus was computed from the formula  $R_0 = 1.2 \, A_3' \times 10^{-13}$  cm.

for the 1S level:

$$\Delta \varepsilon_{10}' = (\Delta E_{10}' / E_0) = (\alpha ZC / 2t)^2 [(\varepsilon t - 3)^2 F_2 + 2 (\varepsilon t - 3) F_4 + F_6 + u^2 (4G_0 - 4\varepsilon tG_1 + \varepsilon^2 t^2 G_2)].$$
(33)

The correction  $\Delta \epsilon_{21}$  for the 2P level is obtained by replacing  $F_m$ ,  $G_m$  by  $F_{m+2}$ ,  $G_{m+2}$  in Eq. (33).

2) The spin-orbit interaction is taken into account by adding to the potential energy the expression

$$\Delta U'' = (2m^2c^2)^{-1}\frac{1}{r}\frac{dU_0}{dr}(LS) = \frac{\alpha^2 Z^2}{2t^2}\frac{1}{x}\frac{dU_0}{dx}\frac{(LS)}{\hbar^2}.$$
 (34)

For the S levels the quantity  $(\mathbf{L}\cdot\mathbf{S})/\hbar^2$  is zero. In the case of the P levels  $(\mathbf{L}\cdot\mathbf{S})/\hbar^2 = -1$  for the  $2P_{1/2}$  sublevel, and  $(\mathbf{L}\cdot\mathbf{S})/\hbar^2 = \frac{1}{2}$  for the  $2P_{3/2}$  sublevel. From Eq. (7) we find

$$\frac{1}{x}\frac{dU_0}{dx} = -\frac{2E_0}{t}, \qquad 0 \leqslant x \leqslant 1,$$
  
$$\frac{1}{x}\frac{dU_0}{dx} = -\frac{2E_0}{tx^3}, \qquad 1 \leqslant x \leqslant \infty.$$
(35)

It is now easy to get the corrections for the spin-orbit interaction for the  $2P_{1/2}$  and  $2P_{3/2}$  sublevels; using the approximate wave functions (21b), (22b), we have:

$$\Delta \varepsilon_{1/2} = -2\Delta \varepsilon_{1/2} = (\alpha^2 Z^2 C^2 / t^3) (F_4 + u^2 G_1).$$
(36)

3) The specific Dirac correction is taken into account by adding to the potential energy the term

$$\Delta U''' = -\left(\frac{\hbar}{2mc}\right)^2 \frac{dU}{dr} \frac{d}{dr} = -\left(\frac{\alpha Z}{2t}\right)^2 \frac{dU}{dx} \frac{d}{dx}.$$
 (37)

Using the fact that U satisfies the Poisson equation

$$\frac{4}{r^2}\frac{d}{dr}\left(r^2\frac{dU}{dr}\right) = 4\pi e\rho\left(r\right),\tag{38}$$

by integrating the expression

$$\int_{0}^{\infty} R(x) \frac{dU}{dx} \frac{dR(x)}{dx} x^{2} dx$$

by parts we can show that the corrections to the energy levels will be given by averaging the nuclear charge density over the wave functions of the states in question\*

$$\Delta E''' = -(\pi e R_0^2 \alpha^2 Z^2 / 2t^2) \int_0^\infty \rho(x) R^2(x) x^2 dx.$$
 (39)

Taking the expression (1) for the charge density and the approximate wave functions (21a), we find for the S levels

$$\Delta \varepsilon_{n0}^{"'} = -(3\alpha^2 Z^2 C^2 / 4t^3) F_2.$$
(40)

The expression for the correction to the P levels is obtained by replacing  $F_2$  by  $F_4$  in Eq. (40).

To give an idea of the accuracy of the approximate calculation of the energy levels of mesic atoms for constant density of the nuclear charge, as made by means of Eqs. (18) and (19) with the relativistic corrections given by Eqs. (34), (36), and (40), there are shown in Table III the energy levels of several  $\mu$ -mesic atoms as found by this method, and also the results of exact (numerical) solution of the Dirac equation.<sup>14</sup> We can also compare the data on the energy levels of  $\mu$ -mesic lead, as obtained by Hill and Ford<sup>7</sup> for constant charge density with  $R_0 = 1.17 \text{ A}^{1/3} 10^{-13} \text{ cm}$  (t = 2.2235), with the results of a calculation by our method:

$$\begin{array}{rrrr} {}^{1S_{\mathbf{i}_{|_{2}}}} & {}^{2P_{\mathbf{i}_{|_{2}}}} & {}^{2P_{\mathbf{i}_{|_{2}}}} \\ 10,620 & 4,809 & 4.623 & \text{according to Hill and Ford} \\ 10,614 & 4,799 & 4,618 & \text{according to our method} \end{array}$$

(the energies are given in Mev). Some part of the difference between our data and those of Hill and Ford is evidently due to the somewhat different values of the constants used in the calculations.

c) <u>The exponential density</u>. Hill and Ford have also made calculations of the energy levels of the mesic lead atom using an exponential density distribution of the charge of the nucleus:

$$\rho(x) = (eZ\delta^3 / 8\pi R_0^3) \exp(-\delta x).$$
(41)

<sup>\*</sup>See also the remark on page 131 of reference 13.

Here  $R_0$  is the radius of the nucleus with constant density, taken as the zeroth approximation, and  $\delta$ is a parameter characterizing the extent of the distribution.  $R_0$  can be chosen, for example, so as to make the mean square radii of the distributions (41) and (1) the same. The potential energy  $U_1$ corresponding to the distribution (41) can be found by integrating the Poisson equation (38):

$$U_1 = (E_0/t) \left[ 2x^{-1} - (2x^{-1} + \delta) \exp(-\delta x) \right].$$
(42)

The difference between  $U_1$  and the potential energy (7) of the zeroth approximation is

$$\Delta U = (E_0 / t) [2x^{-1} - (2x^{-1} + \delta) \exp(-\delta x) - 3 + x^2],$$
  

$$0 \le x \le 1,$$
  

$$\Delta U = -(E_0 / t) (2x^{-1} + \delta) \exp(-\delta x),$$

$$1 \leqslant x \leqslant \infty. \tag{43}$$

In accordance with Eq. (25) we find the correction to the energy  $\epsilon$  of the zeroth approximation for the 1S level by using the approximate wave functions (21a), (22a); with the notations (26a, b, and c) it is:

$$\Delta \varepsilon = (C^2 / t) \{ 2F_1 - 3F_2 + F_4 - e^{-\delta} [2G(\delta, 1; 0, 1) + \delta G(\delta, 2; 0, 1) + 2a^2 G(\delta, 4; 0, 1) + \delta a^2 G(\delta, 5; 0, 1)] + 4aH(\delta, 5) + 2a\delta H(\delta, 7) - u^2 e^{-\delta} [2G(2b + \delta, 1; 1, \infty) + \delta G(2b + \delta, 2; 1, \infty)] \}.$$
(44)

The shift of the 2P level is found by replacing  $F_m$ ,  $G(\xi, m; x_1, x_2)$ , and  $H(\delta, m)$  in Eq. (44) by  $F_{m+2}$ ,  $G(\xi, m+2; x_1, x_2)$ , and  $H(\delta, m+4)$ , respectively.

The results of the calculation by Eq. (44) with inclusion of the relativistic corrections are: 10.458 Mev  $(1S_{1/2})$ , 4.683 Mev  $(2P_{1/2})$ , 4.507 Mev  $(2P_{3/2})$ ; they can be compared with the results of Hill and Ford: 10.504 Mev  $(1S_{1/2})$ , 4.684 Mev  $(2P_{1/2})$ , 4.508 Mev  $(2P_{3/2})$ . The comparatively large discrepancy for the  $1S_{1/2}$  level is explained by the fact that the relativistic corrections for this level are especially sensitive to the

shape of the charge distribution over the volume of the nucleus. From this point of view the exponential distribution is particularly unfavorable for our calculations, since it differs very strongly from the constant distribution, for which the wave functions we used in calculating the relativistic corrections were obtained.

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