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ON THE PROPERTIES OF THE DISCRETE SPECTRUM FOR Z CLOSE TO 137

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The nature of the discrete spectrum for an electron in the Coulomb field of a bare nucleus with charge Z close to 137 is investigated. In this region of Z values the level spectrum significantly depends on the cutoff of the Coulomb potential at small distances. Equation (6) is obtained for the determination of the energy levels ϵ_n. In the logarithmic approximation (i.e., provided that $L = \ln(\hbar/mcR) \gg 1$, where m is the electron mass and R is the nuclear radius), this equation can be solved in explicit form and the simple expressions (24), (25), and (28) are obtained for ϵ_n.

1. INTRODUCTION

It has recently been shown[1-3] that the relativistic Coulomb problem possesses a number of interesting properties. The "collapse to the center," which is well-known from quantum mechanics,[4,5] appears in the Dirac equation for a point charge Ze with Z > 137; as a consequence the energy levels, the S matrix, and the other physical quantities become sensitive to the cutoff of the Coulomb potential $V(r) = -\alpha/r$ at small distances. The introduction of cutoff in the region $r < R$ (i.e., taking the finite size of the nucleus into account) enables us to follow the movement of the levels for $Z > 137$.[6] With an increase of Z the critical value $Z = Z_{cr}(R) > 137$ is attained, at which the ground level $1S_{1/2}$ sinks down to the boundary of the lower continuum, $\epsilon = -mc^2$.

For any cutoff model it is relatively simple to calculate the value of Z_{cr} (see Eq. (8) in article [3]). It is more difficult to obtain an idea about the nature of the entire discrete spectrum in the region of Z values close to 137 because the equation for the energy levels $\epsilon = \epsilon_n(\alpha)$ has a rather cumbersome form (see Eq. (6) below). For this reason, the case of a very small cutoff radius R is considered in the present article, namely, the case when R is not only small compared to the Compton wavelength of the electron, but the more stringent condition (10) is also satisfied. In this approximation, which we shall call the "logarithmic approximation," the problem can be solved in analytic form and the simple formulas (24) and (28) are obtained for the energy levels. It is found that the dependence $\epsilon = \epsilon_n(\alpha)$ has a steplike nature: at that instant ($\alpha = \alpha_{cr}^{(n)}$) when the levels $nS_{1/2}$ and $(n+1)P_{1/2}$ disappear into the lower continuum, all of the levels lying above them abruptly, almost discontinuously, decrease their energy (for more details, see Sec. 3, in particular, Fig. 2).

The question of the accuracy of the logarithmic approximation in the region $R \sim 10^{-12}$ cm (Sec. 3) and the Coulomb problem for a scalar particle (Sec. 6) are also discussed in this article. In Sec. 4 several remarks are made about the application of Case's general method[5] of investigating singular potentials to the present problem. A brief discussion of the obtained results is given in Sec. 7. The Appendix contains a summary of the basic formulas for the Whittaker functions $W_{k,ig}(x)$ which are used in the article.

At the present time there is a great deal of interest in work in the area of the synthesis of superheavy elements. In a number of laboratories searches are being made for elements with Z = 110, 114, and 126; certain isotopes of these elements possess (according to theoretical calculations) a rather large degree of stability with respect to spontaneous fission, α-decay, and β-decay (see the review articles[7,8]). The detection of a nucleus with Z = 110 in cosmic rays was reported in article [9]. There are certain indications[7] of the possible existence of stable nuclei near Z = 164. In this connection, it appears to us that the discussion of the properties of the discrete spectrum for $Z \sim 137$ is rather urgent.

2. THE COULOMB PROBLEM FOR LARGE VALUES OF Z

Let us consider the Dirac equation with the potential[1)]

$$V(r) = \begin{cases} -\alpha/r \text{ for } r > R \\ -\frac{\alpha}{R} f\left(\frac{r}{R}\right) \text{ for } 0 < r < R \end{cases} \quad (1)$$

(R denotes the nuclear radius). In the external region $r > R$ we have the exact solution:

$$G = \sqrt{\frac{1+\varepsilon}{r}}(\chi_1 + \chi_2), \quad F = \sqrt{\frac{1-\varepsilon}{r}}(\chi_1 - \chi_2), \quad (2)$$

where χ_1 and χ_2 are expressed in terms of Whittaker functions (see formulas (12)–(14) in [3]). In the interior region we change to the dimensionless variable $\rho = r/R$ and we take into consideration that $R \ll 1$. Discarding terms of order R, we obtain the following equations for the radial functions G and F:

$$\frac{dG}{d\rho} = -\frac{\varkappa}{\rho}G + \alpha f(\rho)F, \quad \frac{dF}{d\rho} = -\alpha f(\rho)G + \frac{\varkappa}{\rho}F \quad (3)$$

($0 < \rho < 1$). Here, as usual,[10]

$$\varkappa = \mp(j + 1/2) \text{ for } j = l \pm 1/2. \quad (4)$$

1)Here and in what follows, $\alpha = Ze^2/\hbar c = Z/137$. The system of units is used in which $\hbar = c = m = 1$, where m denotes the electron's mass. The remaining notation is the same as in article [3].

In order to determine the spectrum of the levels, it is sufficient to find from (3) only a single constant, which we choose to be the logarithmic derivative of the function G(r) at the edge of the nucleus:

$$\zeta=\left[\frac{r}{G}\frac{dG}{dr}\right]_{r=R}. \quad (5)$$

We note that ζ depends on α, κ, and on the form of the cutoff function $f(\rho)$ (but it does not depend on the energy). The energy level ϵ is found by matching the wave functions at $r = R$. In addition to ζ, the quantities F/G and F′/G for $r \to R-0$, which can be expressed in terms of ζ if ρ is set equal to unity in (3) and it is taken into consideration that $f(1) \neq 1$, appear in the condition for matching. Finally we obtain[2)]

$$xW'_{k,\,ig}(x)\,/\,W_{k,\,ig}(x)=\frac{1}{2}+\zeta-\frac{g^2+\zeta^2}{\alpha t+\varkappa+\zeta}, \quad (6)$$

where $x = 2\lambda R$, $\lambda = \sqrt{1-\epsilon^2}$, $g = \sqrt{\alpha^2-\kappa^2}$, and for the quantities k and t one can take either the values:

$$k=\frac{\varepsilon\alpha}{\lambda}-\frac{1}{2},\quad t=\frac{\lambda}{1+\varepsilon}=\sqrt{\frac{1-\varepsilon}{1+\varepsilon}}, \quad (7a)$$

corresponding to the continuity of χ_1'/χ_1, or else the values

$$k=\frac{\varepsilon\alpha}{\lambda}+\frac{1}{2},\quad t=-\sqrt{\frac{1-\varepsilon}{1+\varepsilon}}, \quad (7b)$$

corresponding to the continuity of χ_2'/χ_2. One can show that for $R \ll 1$ both of these equations are equivalent. We emphasize that Eq. (6) refers to any arbitrary level of the discrete spectrum (with arbitrary values of j, κ, and of the principal quantum number n). For the levels $nS_{1/2}$ ($\kappa = -1$) it goes over into Eq. (16) of article [3] if we set $\zeta = \alpha \cot \alpha$, which corresponds to a square cutoff: $f(\rho) \equiv 1$.

One can solve Eq. (6) by numerical methods if one uses the integral representations given in the Appendix in order to calculate the Whittaker functions. In the following section we shall analyze this equation qualitatively in the limiting case $R \to 0$. Here we only indicate what happens for $\epsilon \to -1$. In this case $t \to \infty$ and on the right-hand side of Eq. (6) one has left $\zeta + 1/2$. Using formula (A.8) from [2], we find

$$zK_{i\nu}'(z)\,/\,K_{i\nu}(z)=2\zeta$$
$$(\nu=2g,\quad z=\sqrt{8\alpha R},\quad \alpha=\alpha_{cr}). \quad (6')$$

We still need to discuss one question of a methodological nature. As follows from (2), as $r \to \infty$ the wave functions with energy ϵ have the following asymptotic form for $-1 < \epsilon < 1$:

$$G=A\sqrt{1+\varepsilon}\,e^{-\lambda r}r^{\alpha\varepsilon/\lambda},\quad F=-A\sqrt{1-\varepsilon}\,e^{-\lambda r}r^{\alpha\varepsilon/\lambda}, \quad (8a)$$

and at the boundary of the lower continuum, $\epsilon = -1$, they have the asymptotic form

$$G=A'(2r/\alpha)^{-1/4}e^{-\sqrt{8\alpha r}},\quad F=-A'(2r/\alpha)^{1/4}e^{-\sqrt{8\alpha r}} \quad (8b)$$

(the constants A and A′ are determined from the normalization). At first glance it is not clear how the asymptotic form (8a) changes into the form (8b). In order to exhibit this, we note that the quasiclassical solution is valid for $r \gg 1$:

$$G,F\propto\exp\{iS(r)\},\quad S(r)=\int_0^r dr\sqrt{\frac{2\alpha\varepsilon}{r}-\lambda^2},$$

where S(r) is the classical action for the radial motion. Let $\epsilon < 0$, then ($r_0 = 2\alpha|\epsilon|/(1-\epsilon^2)$)

$$G(r)\propto\exp\left\{-\lambda\left[\sqrt{r(r+r_0)}+r_0\ln\left(\sqrt{\frac{r}{r_0}}+\sqrt{1+\frac{r}{r_0}}\right)\right]\right\}$$
$$=\begin{cases}\exp(-\sqrt{8\alpha|\varepsilon|r}) & \text{for } r\ll r_0\\ e^{-\lambda r}(r/r_0)^{\alpha\varepsilon/\lambda} & \text{for } r\gg r_0\end{cases}. \quad (9)$$

From here it is clear that the usual asymptotic behavior, $e^{-\lambda r}$, which is characteristic for bound states,[3)] is established only for $r > r_0$. When $\epsilon \to -1$, then the point r_0 goes off to infinity and the opposite condition, $r \ll r_0$, is satisfied; therefore G and F are proportional to $\exp(-\sqrt{8\alpha r})$.

3. THE LOGARITHMIC APPROXIMATION

Equation (6) for the level spectrum has too complicated a form and requires numerical calculations. In order to simplify the situation, let us suppose that $R \to 0$; then the "large logarithm"

$$L=-\ln R\gg 1. \quad (10)$$

appears in the problem. We shall call this approximation the logarithmic approximation, or, more briefly, the L-approximation. First of all let us present some qualitative arguments in favor of the fact that the expansion parameter is L^{-1}.

1) First let $\alpha < 1$. For the ground state of an electron in the field of a point charge Ze we have ($\gamma = \sqrt{1-\alpha^2}$, $\lambda = \alpha$)

$$\varepsilon=\sqrt{1-\alpha^2},$$
$$G(r)=A\sqrt{1+\varepsilon}\,e^{-\lambda r}r^{\gamma},\quad F=-A\sqrt{1-\varepsilon}\,e^{-\lambda r}r^{\gamma}. \quad (11)$$

Using perturbation theory to calculate the levelshift due to the cutoff of the potential in (1), we obtain (for $R \ll 1$)

$$\Delta\varepsilon=\frac{\alpha^2(2\alpha R)^{2\gamma}}{\gamma\Gamma(2\gamma+1)}\left\{1-2\gamma\int_0^1 f(x)x^{2\gamma}dx\right\}. \quad (12)$$

The correction $\Delta\epsilon$ ceases to be small when $R^{2\gamma} \sim 1$, i.e., $\gamma L \sim 1$ or $1-\alpha \lesssim L^{-2}$.

2) Let us estimate the energy of the ground state for $\alpha = 1$ (this value of α is critical for a point charge). In this case the functions G and F have logarithmic singularities at the origin:

$$G(r)\propto r^{\varepsilon}=1+\varepsilon\ln r \text{ for } r\to 0,$$

from which

$$\zeta=[rG'/G]_{r=R}=\varepsilon/(1+\varepsilon\ln R). \quad (13)$$

Since $L \gg 1$ and $\zeta = O(1)$, then $\epsilon(1S_{1/2}) \sim L^{-1}$ for $\alpha = 1$.

3) For $\alpha > 1$ the wave functions in the problem involving the Coulomb potential of a point charge have a singularity of the following type at the origin ($r \ll 1$):

$$G,F\propto\sin(g\ln r^{-1}+\delta),\quad g=\sqrt{\alpha^2-1}. \quad (14)$$

[2)] With regard to the properties of the Whittaker function with an imaginary index, $W_{k,\,ig}(x)$, see the Appendix.

[3)] The factor $r^{\alpha\epsilon/\lambda}$ is due to the interaction of the electron with the nucleus, which (just as in the nonrelativistic case) significantly distorts the wave function at arbitrarily large distances from the nucleus.

For the solutions which decrease at infinity, the phase $\delta = O(g)$ for $\alpha \to 1$. With the cutoff taken into account, formula (14) is valid in the external region $r > R$. Since the wave function of the ground state does not have any nodes, then the $1S_{1/2}$ level may exist only for $gL < \pi$. The maximum possible values of g and α correspond to the disappearance of this level into the lower continuum:

$$g_{cr} = \pi / L, \quad \alpha_{cr} = 1 + \pi^2 / 2L^2. \tag{15}$$

From what has been said it is clear that the parameter L determines both the width of that region around the point $\alpha = 1$, in which it is essential to take the finite size of the nucleus into account, as well as the dependence $\epsilon = \epsilon(\alpha)$ in this range of values of α.

Upon fulfillment of condition (10), by using the asymptotic form (A.2) for the Whittaker function, one can simplify Eq. (6) to the form:

$$(2\lambda R)^{2ig} = \frac{(\zeta + ig)(\alpha t + \varkappa + ig)}{(\zeta - ig)(\alpha t + \varkappa - ig)} \frac{\Gamma(1+2ig)\Gamma(1/2 - k - ig)}{\Gamma(1-2ig)\Gamma(1/2 - k + ig)} \tag{16}$$

Here the specific form of the cutoff enters in a very simple way (only in terms of ζ).

If $\alpha < |\kappa| = j + 1/2$, then $g \to i\gamma$ ($\gamma = \sqrt{\kappa^2 - \alpha^2}$). Provided that $\gamma L \gg 1$ the roots of Eq. (16) are close to the poles of the function $\Gamma(-\epsilon\alpha/\lambda + \gamma)$, appearing in the denominator. This leads to the usual expression for the energy:

$$\varepsilon_{nj} = \left[1 + \frac{\alpha^2}{(n_r + \gamma)^2}\right]^{-1/2}, \quad n_r = n - |\varkappa| = 0, 1, 2, \ldots, \tag{17}$$

which is characteristic of the Coulomb problem with a point charge.

Taking the logarithm of (16) and taking into consideration that $g \ll 1$ according to (15), we obtain

$$\ln 2\lambda R + \frac{1}{g} \arg \Gamma(1/2 - k + ig) = \frac{1}{\zeta} + \frac{1}{\alpha t + \varkappa} + 2\psi(1) - \frac{n'\pi}{g} \tag{18}$$

(n′ is an integer). As $g \to +0$ the function $\omega(x, g) = \Gamma(x + ig)$ experiences abrupt discontinuities near the points $x = -n$ at which the poles of the Γ function are located. Namely, if $|x + n| \gg g$, then to within terms of order g^2 one has

$$\omega(x, g) = \begin{cases} g\psi(x) & \text{for} \quad x > 0 \\ -(n+1)\pi + g\psi(x) & \text{for} \; -(n+1) < x < -n \end{cases} \tag{19}$$

where $\psi(x)$ denotes the logarithmic derivative of the Γ-function. In the immediate vicinity of the pole $x = -n$ one has

$$\omega(x, g) = -\left(n\pi + \operatorname{arc\,ctg} \frac{x+n}{g}\right). \tag{19′}$$

In the region $1 \gg |x + n| \gg g$ formulas (19) and (19′) are matched to each other, and both expressions give

$$\omega(x, g) = -[(n + \nu)\pi + g / (x + n) + \ldots], \tag{19″}$$

where $\nu = 0$ for $x > -n$ and $\nu = 1$ for $x < -n$. We further note that $\omega(x, g)$ is a monotonically increasing function of x (for arbitrary $g > 0$) since

$$\omega'(x, g) = \operatorname{Im} \psi(x + ig) = g \sum_{k=0}^{\infty} \left[(x+k)^2 + g^2\right]^{-1} > 0. \tag{19‴}$$

Now one can write down the solution of Eq. (16) in explicit form. First let us assume that $\epsilon = -1$. Then $1/2 - k \to \infty$ (see Eq. (7)) and from Eqs. (18) and (19) we obtain

$$g_{cr} = \frac{n'\pi}{L - \ln(2j+1) + 2\psi(1) + \zeta^{-1}} \tag{20}$$

$$\alpha_{cr} = j + \frac{1}{2} + \frac{(n'\pi)^2}{(2j+1)L^2} + O(L^{-3}) \tag{21}$$

Here $n' = 1, 2, 3, \ldots$; $\psi(1) = -0.5772$ (Euler's constant). In what follows we shall relate n′ with κ and with the principal quantum number n. We note that α_{cr} depends on the sign of κ only by means of ζ. Since we are interested in the region $\alpha \approx 1$, then it is sufficient to consider states of the type $S_{1/2}$ and $P_{1/2}$ ($\kappa = \mp 1$) since for all remaining levels α_{cr} is too large and for $\alpha < 2$ one can use formula (17) for them, this formula referring to the Coulomb potential of a point charge. In the field of a point charge with $\alpha < 1$ the states $nS_{1/2}$ and $nP_{1/2}$ are degenerate with respect to the energy; as $\alpha \to 1$

$$\varepsilon_n = \frac{n-1}{(n^2 - 2n + 2)^{1/2}} + \frac{\gamma}{(n^2 - 2n + 2)^{3/2}} + O(\gamma^2). \tag{22}$$

For $n = 1$ this formula describes the nondegenerate ground level $1S_{1/2}$, and for $n \geq 2$ it describes the states $nS_{1/2}$ and $nP_{1/2}$. Expression (22) has a square-root singularity at the point $\alpha = 1$, and therefore it cannot be directly continued into the region $\alpha > 1$.

If quantities of the order of unity[4)] are neglected in comparison with quantities of the order of L, and if we do not yet consider the case $\epsilon \to -1$ (when $\ln \lambda$ cannot be neglected in comparison with L), then the equation for the energy levels takes the following simple form:

$$\omega(-\varepsilon / \lambda, g) = gL - n\pi \text{ for } \varkappa = -1, \tag{23a}$$

$$\omega(1 - \varepsilon / \lambda, g) = gL - (n-1)\pi \text{ for } \varkappa = +1, \tag{23b}$$

where n denotes the principal quantum number, and $\omega(x, g)$ is the function defined above. In this connection, the number n′ appearing in Eq. (20) is given by $n' = n - (1 + \kappa)/2$. With (19′) taken into account, from here we obtain the following result for the ground state energy:

$$\varepsilon_1(\alpha) = \begin{cases} \gamma \operatorname{cth} \gamma L & \text{for } \alpha \leqslant 1 \\ g \operatorname{ctg} gL & \text{for } \alpha \geqslant 1 \end{cases}. \tag{24}$$

We recall that $\gamma = \sqrt{1 - \alpha^2}$ and $g = \sqrt{\alpha^2 - 1}$. In contrast to (22) the point $\alpha = 1$ is not singular for $\epsilon_1(\alpha)$. In the region $\alpha < 1$ (i.e., up to the "collapse to the center" $\coth \gamma L \to 1$ and even for $L^2(1 - \alpha) \gg 1$ the energy $\epsilon_1(\alpha)$ essentially does not depend on the cutoff of V(r) (see Fig. 1), and (24) goes over into the corresponding formula for a point charge, $\epsilon_1(\alpha) \to \sqrt{1 - \alpha^2}$.

For $\alpha > 1$ the function (24) has a pole for $g = g_{cr} = \pi/L$. Indeed, it is clear that $\epsilon_1(\alpha_{cr}) = -1$ but not $-\infty$. The point is that the approximation (23) ceases to be valid when $\epsilon_1(\alpha)$ is not small. For $g - g_{cr} \sim L^{-2}$ there exists a region of rapid decrease of the energy ϵ_1 from values close to zero to the boundary $\epsilon = -1$. We shall investigate it a little bit later on (see Eq. (28)).

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4) In this connection we automatically neglect the splitting of the levels $nS_{1/2}$ and $nP_{1/2}$ which is of the order of $(\zeta_+ - \zeta_-)L^{-2}$. In this approximation the energy levels do not depend on the shape of the cutoff of the potential inside the nucleus.

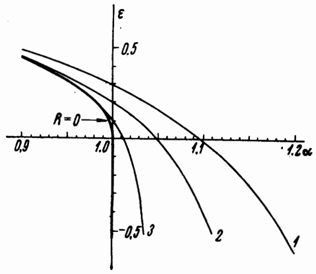

FIG. 1. The ground state energy $\epsilon_1(\alpha)$ for values of α close to unity. Curves 1, 2, and 3 correspond to L = 3.5, 5, and 10 (the corresponding values of the cutoff radius R are equal to 12, 2.6, and 0.018F). The limiting curve for R = 0 (the point Coulomb potential) has a square-root singularity at $\alpha = 1$, and then goes vertically downwards.

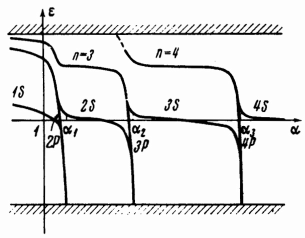

FIG. 2. The energies of the lower levels of the discrete spectrum near $\alpha = 1$ (the qualitative form of $\epsilon_n(\alpha)$ for $L \gg 1$); $\alpha_n = 1 + n^2\pi^2/2L^2$ denotes the critical value α_{cr} for the levels $nS_{1/2}$ and $(n+1)P_{1/2}$.

Let us summarize. An electron in the state with $j = 1/2$ begins to "experience" the singularity of the Coulomb potential as $r \to 0$ when α approaches the critical value $\alpha_{cr}(0) = 1$ (for a point charge, R = 0) at a distance of the order of L^{-2} (see Fig. 1). We note that the difference $\alpha_{cr}(R) - 1$ is also of the order of L^{-2}, that is, all phenomena associated with the "collapse to the center" take place in the region $\Delta\alpha \sim L^{-2}$ around the point $\alpha = 1$. In this connection, as long as $g_{cr} - g \gg L^{-2}$ (or, what is the same thing, $\alpha_{cr} - \alpha \gg L^{-3}$), the energy of the ground state is described by formula (24).

Now let us go on to the excited levels ($n \geq 2$, $\kappa = \pm 1$). For them one will have $\epsilon/\lambda \to n - 1$ as $\alpha \to 1$. Therefore the approximation (19′) is valid for the ω-function in (23), and this gives

$$\varepsilon_n(\alpha) = \frac{n-1}{(n^2-2n+2)^{1/2}} + \frac{g \operatorname{ctg} gL}{(n^2-2n+2)^{3/2}}. \tag{25}$$

This expression remains valid even for $\alpha < 1$ provided we make the substitution $g \to i\gamma$. Taking the cutoff of the Coulomb potential into account changes formula (22) for a point charge only with regard to $\gamma \to \gamma \coth \gamma L$. This correction rapidly becomes unimportant as the value of α decreases; however in the region $|\alpha - 1| \sim L^{-2}$ around the point $\alpha = 1$ it has a decisive value. According to Eq. (25) the energies of all levels decrease monotonically with increasing α. For $g = g_{cr} = \pi/L$ the $1S_{1/2}$ and $2P_{1/2}$ levels disappear into the lower continuum, and the remaining levels undergo a shift: $n \to n - 1$, after which the level spectrum is again described by formula (25). The next abrupt change in the spectrum occurs for $g = 2\pi/L$, when the levels $2S_{1/2}$ and $3P_{1/2}$ disappear into the lower continuum, and so forth. With an increase of α, such abrupt changes may be repeated many times (see Fig. 2) as long as, finally, we do not escape from the region $g \ll 1$.

The entire region $\alpha > 1$ is subdivided into regions corresponding to slow and rapid changes of the level spectrum. The "slow" regions correspond to $(n-1)\pi/L < g < n\pi/L$, where g is separated from the end points of this interval by an amount $\gtrsim L^{-2}$; here formulas (24) and (25) are applicable. The "rapid" regions consist of the intervals $\Delta g \sim L^{-2}$ around the critical points $g = g_{cr}^{(n)} = n\pi/L$. In order to obtain the equation for $\epsilon(\alpha)$ in this case, it is necessary to return to Eq. (18) and to take into consideration that the Γ-function is not close to a pole, and therefore one can use formula (19) for $\omega(1/2 - k, g)$. Ultimately we find (for $\epsilon > 0$)

$$\psi(-\varepsilon/\lambda) = \pi^{-1}L(gL - n\pi). \tag{26}$$

The curve $\epsilon = \epsilon(\alpha)$, determined by this equation, joins smoothly with (25). Let us demonstrate this for the example of the $2S_{1/2}$ level, whose energy is given by

$$\varepsilon_2(\alpha) = \begin{cases} 2^{-1/2}[1 - \pi/2L(\pi - gL)] & \text{for } gL < \pi \\ g \operatorname{ctg} gL & \text{for } \pi < gL < 2\pi \end{cases} \tag{27}$$

Under the condition $1 \gg |gL - \pi| \gg L^{-1}$, from here we find

$$\varepsilon_2(\alpha) = \begin{cases} 2^{-1/2}\left[1 + \frac{g}{2} \operatorname{ctg} gL\right] & \text{for } 0 < gL < \pi \\ g \operatorname{ctg} gL & \text{for } \pi < gL < 2\pi \end{cases} \tag{27′}$$

On the other hand, the argument of the ψ-function in Eq. (26) changes from −1 to 0, and if it is taken into consideration that near the pole $(z \to -n)$

$$\psi(z) = -(z+n)^{-1} + \psi(n+1) + O(z+n),$$

then from (26) we obtain the same expression as above for $\epsilon_2(\alpha)$.

We still have to investigate the behavior of the levels in the region $\epsilon \geq -1$, which is immediately adjacent to the lower continuum. Here in Eq. (18) it is necessary to retain the $\ln \lambda$, which is important as $\epsilon \to -1$. With the aid of (20) we can eliminate from (18) the terms which depend on ζ, after which the equation for ϵ takes the form

$$f_\pm(\varepsilon) = L(1 - g/g_{cr}), \qquad g_{cr} = n'\pi/L. \tag{28}$$

For the $nS_{1/2}$ levels we have: $\kappa = -1$, $0 > \epsilon \geq -1$, $n' = n$, and

$$f_-(\varepsilon) = -\left[\ln \lambda + \psi\left(-\frac{\varepsilon}{\lambda}\right) + \frac{1+\varepsilon}{1+\varepsilon+\lambda}\right], \tag{29a}$$

and for the $nP_{1/2}$ levels one has: $\kappa = +1$, $n' = n - 1$, $2^{-1/2} > \epsilon \geq -1$, and

$$f_+(\varepsilon) = -\left[\ln \lambda + \psi\left(1-\frac{\varepsilon}{\lambda}\right) - \frac{1+\varepsilon}{1+\varepsilon+\lambda}\right]. \tag{29b}$$

We note that as $\epsilon \to -1$

$$f_+(\varepsilon) = {}^2/_3(1+\varepsilon) + \ldots, \quad f_-(\varepsilon) = {}^5/_3(1+\varepsilon) + \ldots \tag{30}$$

From here it follows that as $\alpha \to \alpha_{cr}$ the levels disappear into the lower continuum, having a finite derivative $(\partial\epsilon/\partial\alpha)$:

$$\varepsilon_n^{\pm}(\alpha) = -1 + \frac{c_\pm L^3}{n'^2}(\alpha_{cr} - \alpha) \tag{31}$$

($c_+ = 3/2\pi^2$, $c_- = 3/5\pi^2$). For $L \gg 1$ and for small values of n the curve $\epsilon = \epsilon(\alpha)$ becomes very steep: almost all of the change of ϵ from 0 (or $2^{-1/2}$) to −1 takes place in the region $\Delta\alpha \sim L^{-3}$ near α_{cr}. For highly-excited states ($n \gg 1$) this sharp decrease is smoothed out. At the other end of the interval under consideration, expressions (28) and (29) join smoothly with (25). For example, for n = 1 (the ground state) under the assumption that $g_{cr} \gg g_{cr} - g \gg g_{cr}^2$ both (24) and (28) give

$$\varepsilon_1(\alpha) = -g_{cr}^2/\pi(g_{кр} - g) = -\pi/L(\pi - gL) \qquad (32)$$

(here $g_{cr} = \pi/L$, $1 \gg |\epsilon_1| \gg L^{-1}$). The dependence $\epsilon = \epsilon(\alpha)$ which is determined by Eq. (28) is shown in Fig. 3. For purposes of comparison, the corresponding curve for a scalar particle is also shown.

In addition to the spectrum of the levels, it is also of interest to determine the form of the wave functions as $\alpha \to 1$. In order to not have to present cumbersome formulas, we shall confine our investigation to the ground state. In analogy with (11) we assume

$$G = \sqrt{1+\varepsilon}e^{-x/2}x^{\varepsilon}[1 - (\varepsilon^2 + g^2)\xi_1(x) + \ldots],$$
$$F = -\sqrt{1-\varepsilon}e^{-x/2}x^{\varepsilon}[1 - (\varepsilon^2 + g^2)\xi_2(x) + \ldots] \qquad (33)$$

($x = 2\lambda r$; ϵ, $g \to 0$). Substituting these expansions into the Dirac equation, we obtain the following equations for the corrections ξ_1 and ξ_2:

$$\xi_1' - \left(\frac{1}{2} + \frac{1}{x}\right)(\xi_1 - \xi_2) = \frac{1}{2x},$$
$$\xi_2' + \left(\frac{1}{2} - \frac{1}{x}\right)(\xi_1 - \xi_2) = -\frac{1}{2x}. \qquad (34)$$

The solution of this system (vanishing at infinity) has the form

$$\xi_{1,2}(x) = \int_0^\infty dt\, e^{-xt}\left\{\frac{\ln(1+t)}{t} \mp \frac{1}{2(1+t)}\right\}, \qquad (35)$$

where

$$\xi_{1,2}(x) = {}^1/_2 \ln^2 x + O(\ln x) \text{ as } x \to 0,$$
$$\xi_1 = 1/2x + \ldots, \quad \xi_2 = 3/2x + \ldots \text{ as } x \to \infty. \qquad (36)$$

The condition for the applicability of the expansion (33) is $(\epsilon^2 + g^2)|\xi(x)| \ll 1$, or $x \gg x_0 = \exp\{-(\epsilon^2 + g^2)^{-1/2}\}$. Here $\epsilon = g \cot gL$; therefore $x_0 \sim R$ for $\alpha > 1$, but for $\alpha < 1$ the quantity $x_0 = \exp\{-\gamma^{-1} \sinh \gamma L\}$ rapidly tends to zero, and the difference between the wave functions (33) and expressions (11), which are characteristic of a point charge, becomes small for all values of r. We further note that in the region $x_0 \ll x \ll 1$ (when $g \ln r \gg 1$)

$$G \approx -F = 1 + \varepsilon \ln x - {}^1/_2 g^2 \ln^2 x + \ldots \qquad (37)$$

In concluding this section, let us say a few words about the accuracy of the L-approximation in the actual domain corresponding to the radii of heavy nuclei, $R \approx 10^{-12}$ cm (L = 3 to 4). For this purpose let us compare the critical values α_{cr} obtained by the numerical solution of Eq. (6′) with the asymptotic formulas (20) and (21). As always happens in such cases, the problem arises about the choice of the best asymptotic form, since expressions which do not differ among themselves in the limit $L \to \infty$ give different numerical results for small values of L. For example, the calculation according to formula (21) leads to an error ~40% in the value of $\alpha_{cr} - 1$. On the other hand, the more fundamental (with regard to its derivation) relation (20) has better accuracy. Let us introduce the notation

$$\sigma_1 = Lg_{cr}/\pi, \quad \sigma_2 = (L - \ln 2 + 2\psi(1) + \zeta^{-1})g_{cr}/\pi \qquad (38)$$

(the deviation of the quantities σ_1 and σ_2 from unity characterizes the accuracy of the L-approximation). From Fig. 4 it is seen that the simplest formula $g_{cr} = \pi/L$ gives g_{cr} with an excess, but taking account of the correction terms in (20), which depend on the cutoff,

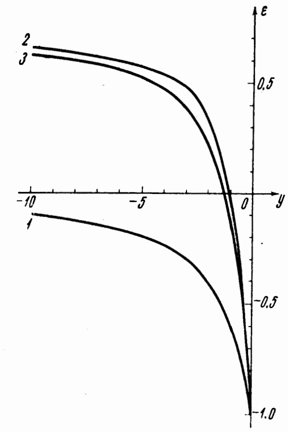

FIG. 3

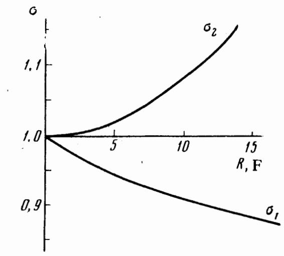

FIG. 4

FIG. 3. The dependence of the energy level ϵ on α in the region of "rapid collapse" associated with $\alpha \to \alpha_{cr}$. Curves 1 and 2 refer to the levels $1S_{1/2}$ and $2P_{1/2}$, and curve 3 refers to the 1S level for a particle with zero spin. The quantity $y = L(g-g_{cr})/g_{cr}$ is plotted along the axis of abscissas.

FIG. 4. The question of the accuracy of the L-approximation. The curves refer to the lowest level $1S_{1/2}$ for model I (a square cutoff, see [2]). The values of the cutoff radius R are given in fermis.

improves the accuracy in the region of small values of R and gives an approximation with a shortage. On the whole (20) determines g_{cr} with an accuracy ~10%.

The small differences between the values of α_{cr} for the $nS_{1/2}$ and $(n+1)P_{1/2}$ levels are also described by formula (20), but with worse accuracy:

$$\Delta\alpha_n = \alpha_{cr}((n+1)P_{1/2}) - \alpha_{cr}(nS_{1/2}) \approx \frac{n^2\pi^2(\zeta_+ - \zeta_-)}{L^3\zeta_+\zeta_-}. \qquad (39)$$

One can show that ζ_+ is always greater than ζ_-, and therefore $\Delta\alpha_n > 0$. Numerically, for R = 10 F and n = 1, expression (39) gives $\Delta\alpha_1 = 0.20$, which exceeds the true value $\Delta\alpha_1 = 0.11$ by almost a factor of two.

4. COMMENT ON CASE'S METHOD

In addition to the explicit introduction of a cutoff for $r < R$, there is another method for investigating singular potentials in quantum mechanics, which is based on the choice of the boundary conditions at the origin (see [5, 11]). The Dirac equation with the potential $V(r) = -\alpha/r$ is now considered over the entire space $0 < r < \infty$. For $r \to 0$, by neglecting the nonsingular terms we obtain the system of equations

$$rG' = -\varkappa G + \alpha F, \qquad rF' = -\alpha G + \varkappa F, \qquad (40)$$

whose solutions have the form $r^{\pm\gamma}$. As long as $\alpha < |\kappa|$, one can choose the less singular solution from these solutions and, by following [4], it is not difficult to show that it is precisely this solution which is of physical significance.

For $\alpha = |\kappa|$ the regular solution is finite at the origin:

$$G(0)/F(0) = \operatorname{sign}\varkappa, \qquad (41a)$$

but the singular solution has a logarithmic singularity:

$$G(r) = \ln r - \frac{1}{2\varkappa} + \ldots, \quad F(r) = \left(\ln r + \frac{1}{2\varkappa} + \ldots\right)\operatorname{sign}\varkappa. \qquad (41b)$$

Finally, if $\alpha > |\kappa|$, then $\gamma = ig$, and both solutions are identically acceptable. In this case ($r \to 0$)

$$G = \sin(g \ln r + \beta), \quad F = \sin(g \ln r + \beta + \psi), \tag{42}$$

where β is an arbitrary constant, but the phase shift ψ between F and G is quite definite:

$$e^{i\psi} = \frac{\varkappa + ig}{\alpha}, \quad \psi = \arccos\frac{\varkappa}{\alpha} \quad (g = \sqrt{\alpha^2 - \varkappa^2}). \tag{43}$$

The physical meaning of β consists in the fact that it is the phase of the wave which is reflected from the singular point $r = 0$ (see article [11], in which this constant is denoted by γ, for more details). The choice of the boundary condition at the origin reduces to the choice of β in (42). After this the spectrum of the energy levels ϵ is uniquely determined, the wave functions for different points $\epsilon_1 \neq \epsilon_2$ of the spectrum are mutually orthogonal, and the system of eigenfunctions is complete.[5]

The parameter β contains all the information about the nature of the cutoff of the potential at small distances which is needed in order to determine the energy level spectrum. In fact, from Eqs. (5) and (42) we find

$$\zeta = g \operatorname{ctg}(g \ln R + \beta), \quad \beta = gL + \operatorname{arc\,tg}(g/\zeta). \tag{44}$$

In order to determine the discrete spectrum, we note that a solution which vanishes at infinity (see Eq. (2)) exists for any value of ϵ in the interval $-1 \le \epsilon < 1$. For $r \to 0$ it has the form (42) with a definite phase $\beta = \beta(\epsilon, \alpha, \kappa)$ which one can find by solving the Dirac equation:

$$\beta = g \ln 2\lambda - \arg\left\{\left(\alpha\sqrt{\frac{1-\varepsilon}{1+\varepsilon}} + \varkappa + ig\right) \times \Gamma(1 + 2ig) \Big/ \Gamma\left(1 - \frac{\alpha\varepsilon}{\lambda} + ig\right)\right\} \tag{45}$$

(this expression simplifies somewhat for $\epsilon = -1$: $\beta = g \ln 2\alpha - \arg\Gamma(1 + 2ig)$). Equating expressions (44) and (45), we obtain the transcendental equation which determines the discrete spectrum. Let us consider it in the L-approximation for $\kappa = \pm 1$. Then ($N = (n^2 - 2n + 2)^{1/2}$)

$$\varepsilon_n(\alpha) = \frac{n-1}{N} + \frac{g \operatorname{ctg}\beta}{N^3} + \ldots \tag{46}$$

If here β is formally regarded as a quantity that does not depend on α, then ϵ_n as a function of α will have a singularity for $\alpha = 1$, and also for $\alpha > 1$ the energy ϵ_n may either decrease with increasing values of α or else increase depending on the sign of $\cot\beta$.

Such an ambiguity was considered earlier[5] as a definite difficulty of the given method. However, in any cutoff model, $\beta \sim gL$ for $\alpha \to 1$ and $L \gg 1$, and (46) goes into (25). This indicates that for $R \ll 1$ Case's method leads to the same results as the direct cutoff of the potential in the region $r < R$. It is only necessary to take into consideration that the phase β, which has been introduced in a formal manner, is in fact uniquely associated with ζ and R. We note that one can also obtain formula (20) for g_{cr} by using this method.

5. CONCERNING THE POSITRON LEVELS

Usually the levels of the discrete spectrum emerge from the upper continuum. The specific Coulomb problem is then such that in this case for $\epsilon = -1$ there is always a wave function which is decreasing at infinity:

$$G(r) = \alpha K_\tau(\sqrt{8\alpha r}), \quad F(r) = (\varkappa + \gamma) K_\tau(\sqrt{8\alpha r}) - \sqrt{2\alpha r} K_{\tau+1}(\sqrt{8\alpha r}) \tag{47}$$

(here $\tau = 2\gamma = 2\sqrt{\kappa^2 - \alpha^2}$; for $\alpha > |\kappa|$ we have $\tau = i\nu = 2ig$). For $r \to \infty$ the functions G and F decrease as indicated in (8b), but for $r \to 0$

$$G \propto r^{-\gamma}, \quad F/G = (\varkappa - \gamma)/\alpha. \tag{47'}$$

For $\gamma < 1/2$ (that is, for $\alpha > \sqrt{j(j+1)}$) the normalization integral

$$\int_0^\infty (G^2 + F^2)\,dr$$

converges, and the question arises as to the possible existence of positron levels. Such levels would emerge from the lower continuum and would correspond to bound states of the positron.[5)] Even though $V(r) = \alpha/r > 0$ for positrons, the effective potential $U_{eff}(r)$ gives an attraction at small distances due to the term $-\frac{1}{2}V^2$, and therefore such levels may arise in principle. It is impossible to clarify the question about the existence of positron levels by working with the point Coulomb potential. Just like earlier we cut off $V(r)$ for $r < R$ and only in the final answer do we let R tend to zero. For the determination of those values of α at which a bound state of the electrons exists with $\epsilon = -1$ (i.e., a positron level with zero binding energy), we have Eq. (6′) in which $i\nu \equiv \tau$.

First let $\alpha < |\kappa|$. Then τ is real, and therefore for $z > 0$

$$z\frac{K_\tau'(z)}{K_\tau(z)} = -\left[z\frac{K_{\tau-1}(z)}{K_\tau(z)} + \tau\right] < -\tau < 0.$$

On the other hand, one can show[6)] that $\zeta > \sqrt{\kappa^2 - \alpha^2} > 0$. Hence it follows that for $\alpha < |\kappa|$ Eq. (6′) does not have any solutions. However, if $\alpha > |\kappa|$ then solutions appear for the critical values $\alpha = \alpha_{cr}$ of the coupling constant. In connection with a small change $\alpha = \alpha_{cr} + \Delta\alpha$ the energy level is changed by the amount $\Delta\epsilon = -\beta\Delta\alpha$, where $\beta > 0$ (see formula (29) in [2]). Therefore, for $\alpha > \alpha_{cr}$ the level under consideration withdraws into the lower continuum (a positron level would move upwards, i.e., it would correspond to $\beta < 0$).

One can make an even more general statement about the behavior of the curve $\epsilon = \epsilon(\alpha)$ for an arbitrary level. Namely, let $V(r) = -\alpha v(r)$ where α is the coupling constant, and $v(r) \ge 0$ is any non-negative function (the cutoff Coulomb potential (1) belongs to this type). Calculating the level shift by using perturbation theory, we find

$$\frac{\partial\varepsilon}{\partial\alpha} = -\int_0^\infty v(r)\{G^2(r,\varepsilon) + F^2(r,\varepsilon)\}\,dr < 0 \tag{48}$$

[5)] The Dirac equation is invariant under the substitutions: $\epsilon \to -\epsilon$, $V(r) \to -V(r)$, $\kappa \to -\kappa$, $G \rightleftharpoons F$; therefore the level with $\epsilon = -1$ for an electron corresponds to a positron level with zero binding energy. A. B. Migdal called our attention to the necessity of investigating the question of positron levels.

[6)] The logarithmic derivative ζ at the edge of the nucleus decreases with increase of the function $f(\rho)$. For an arbitrary distribution inside the nucleus $f(\rho) < \rho^{-1}$, and Eqs. (3) for $f(\rho) = \rho^{-1}$ have the exact solution: $G = \rho^\gamma$, $F/G = (\kappa + \gamma)/\alpha$ for which $\zeta = \gamma = \sqrt{\kappa^2 - \alpha^2}$.

(here G and F are the exact wave functions of the level with energy ϵ). From here it is seen that with increasing α the curve $\epsilon = \epsilon(\alpha)$ falls monotonically, which corresponds to an electron level but not to a positron level. For Coulomb potentials V(r) with a Coulomb tail at infinity, $F^2 + G^2$ is quadratically integrable not only for $-1 < \epsilon < 1$ but also for $\epsilon = -1$; therefore the level $\epsilon(\alpha)$ moves off into the lower continuum, having a finite derivative $\partial\epsilon/\partial\alpha$.

Thus, bound states of positrons are not present in the Coulomb field (1) (at any rate, not within the framework of the single-particle approximation).

6. THE COULOMB PROBLEM FOR A SCALAR PARTICLE

Let us consider a particle with zero spin in a Coulomb field. For $\alpha < 1/2$ the Klein–Gordon equation has the solution (for a point charge)

$$\chi_0(r) = e^{-\lambda r} r^{\sigma},$$

$$\lambda = (1/2 - \sqrt{1/4 - \alpha^2})^{1/2}, \quad \sigma = 1/2 + \sqrt{1/4 - \alpha^2}.$$

This wave function[7] corresponds to the lowest level n = 1, $l = 0$; its energy is given by $\epsilon_1 = \sqrt{\sigma}$. For $\alpha > 1/2$ it is necessary to introduce a cutoff of the potential V(r).

As long as $\alpha < 3/2$, only the s-states, which we therefore consider, experience a strong perturbation. The energy level is determined from the equation[3]

$$xW'_{k,ig}(x)/W_{k,ig}(x) = \zeta$$
$$(x = 2\lambda R, \quad k = \varepsilon\alpha/\lambda, \quad g = \sqrt{\alpha^2 - 1/4}) \tag{49}$$

Hence in the L-approximation $k - 1/2 = g \cot gL$, and for the energy of the ground state we find

$$\varepsilon_1 = [1/2 + g \operatorname{ctg} gL]^{1/2} \approx 2^{-1/2}[1 + g \operatorname{ctg} gL]. \tag{50}$$

When $g \to g_{cr} = \pi/L$ ($\alpha \to \alpha_{cr} = 1/2 + \pi^2 L^{-2}$) the lowest level rapidly falls to $\epsilon = -1$. Its motion in this range of values of α is determined by an equation of the type (28), in which it is necessary to replace $f_{\pm}(\epsilon)$ by

$$f_0(\varepsilon) = -\left[\ln 2\lambda + \psi\left(\frac{\lambda - \varepsilon}{2\lambda}\right)\right].$$

See the corresponding curve in Fig. 3. From a comparison with Section 3 it is obvious that the nature of the dependences of ϵ on α are identical for spin 0 and spin $1/2$ (the relativistic Coulomb potential does not distinguish between bosons and fermions).

Finally we note that Eq. (49) simplifies considerably for $\epsilon = 0$ and $\epsilon = -1$. In the first case, according to Eq. (A.9) we obtain

$$RK_{ig}'(R) = (\zeta - 1/2)K_{ig}(R) \quad (\varepsilon = 0), \tag{51}$$

and for $\epsilon = -1$ we have

$$zK_{i\nu}'(z) = (2\zeta - 1)K_{i\nu}(z) \quad (\nu = 2g = \sqrt{4\alpha^2 - 1}, \quad z = \sqrt{8\alpha R}); \tag{52}$$

In Eqs. (51) and (52) the quantity α is unknown.

7. DISCUSSION OF THE RESULTS

Let us make several concluding remarks.

1. For $\alpha = 1$ the Coulomb problem for a point charge loses its meaning since the energy levels with $\kappa = \pm 1$ have a square-foot singularity at the point $\alpha = 1$ and upon formal continuation into the region $\alpha > 1$ they become complex. Therefore, it is necessary to introduce, by one method or another, a cutoff of the potential $V(r) = -\alpha/r$ for $r < R$; after this is done the problem becomes mathematically "proper," and one can investigate the motion of the levels with increasing values of α.[8]

2. Although values $R \approx 10^{-12}$ cm ($R \sim 0.03$ in units of $\hbar/mc$) have a direct physical significance, in principle the radius R of the cutoff may be arbitrarily small. This makes it possible to seek the level spectrum in the L-approximation (see condition (10)). Numerically, the parameter L^{-1} is still not very small in the region $R \sim 10^{-12}$ cm, but such an approximation is sufficient to obtain a qualitative picture of the motion of the levels.

3. The situation associated with the "collapse to the center" in the relativistic equations for spin 0 and spin $1/2$ particles differs from ordinary quantum mechanics in two respects. If $V(r) = -\alpha r^{-n}$ as $r \to 0$, then a "collapse to the center" arises in the nonrelativistic case[4] for $n \ge 2$ and for positive values of α (more accurately, for $\alpha > 1/4$), whereas in the relativistic case it is sufficient to have $n \ge 1$ and the sign of α may be arbitrary. Formally this is accounted for by the fact that $U_{eff}(r) \sim -1/2 V^2$ as $r \to 0$, and the physical reason is that the Dirac and Klein-Gordon equations with vector coupling simultaneously describe particles and antiparticles. Therefore, the introduction of a cutoff radius R into the Coulomb field with $Z > 137$ is necessary not only for electrons but also for positrons (in spite of the fact that the latter are repelled by the nucleus).

4. An electron in the state with total angular momentum $j = 1/2$ begins to experience the singularity of the Coulomb potential when $1 - \alpha$ becomes comparable with L^{-2}. This is true not only for the lowest level $1S_{1/2}$, but also for all of the higher excited states $nS_{1/2}$ ($\kappa = -1$) and $nP_{1/2}$ ($\kappa = +1$) whose energies for $n \gg 1$ still lie in the nonrelativistic region:

$$\varepsilon_n^{\pm} = 1 - \frac{1}{2n^2} - \frac{1 - g \operatorname{ctg} gL}{n^3} + \ldots \tag{53}$$

It may seem strange that the levels with $n \gg 1$ for $\alpha \to 1$ are sensitive to the cutoff of the potential for $r < R \ll 1$. The reason is that for all states with $j = 1/2$ the effective potential in the Dirac equation behaves like $(3/4 - \alpha^2)r^{-2}$ as $r \to 0$, that is, the "collapse to the center" begins for $\alpha > 1$. Since $\epsilon_{n+1} - \epsilon_n \approx n^{-3}$, then the level shift due to the finite size of the nucleus is much smaller than the distance between neighboring levels so long as $gL < \pi$. When $g \to g_{cr} = \pi/L$, the energies ϵ_n rapidly change with increase of α. In this connection the $1S_{1/2}$ and $2P_{1/2}$ levels disappear into the lower continuum, but for all remaining states with $\kappa = \mp 1$ the picture seems to be as if the principal quantum number were decreased by unity: $n \to (n-1)$. With a further increase of α, these phenom-

[7] For the ground state in the Coulomb potential with a point charge, we have $k = \sigma$, $ig = \sigma - (1/2)$, and the wave function $W_{k,\,ig}(2\lambda r)$ simplifies appreciably as a consequence of the identity (A.4).

[8] Actually we have everywhere regarded α as a continuous variable. This is permissible since according to Eq. (21) the difference $Z_{cr}(R) - 137$ becomes smaller than unity only for $R < \exp\{-\pi\sqrt{\hbar c/2e^2}\} \sim 10^{-22}$ cm.

ena are repeated. The energy of each separately taken level monotonically falls with increasing α, and the discrete spectrum as a whole changes periodically together with g (with the period $\Delta g = \pi/L$).

The step-like shape of the curve $\epsilon = \epsilon(\alpha)$ with the division into segments corresponding to rapid and slow variation is preserved so long as $g = \sqrt{\alpha^2 - 1} \ll 1$. With a further increase of α this curve is smoothed out. The levels $nS_{1/2}$ and $nP_{1/2}$ remain almost degenerate so long as $g < (n-1)\pi/L$; however, the values of g_{cr} for them are different (see formula (20) and Fig. 2).

5. Taking the finite size of the nucleus into account gives corrections to the energy levels which are essential for $\alpha \to |\kappa|$. The structure of these corrections is the same in all of the cases which were considered (compare formulas (24) and (25) for spin $s = 1/2$ and formula (50) for $s = 0$).

6. The disappearance of levels into the lower continuum raises a number of questions of both a mathematical and physical nature. The mathematical question is whether the system of eigenfunctions remains complete for $g > g_{cr}$ (and all the more for $g > g_{cr}^{(n)} = n\pi/L$, when n levels have disappeared into the lower continuum). Although this question certainly deserves a more detailed investigation, it appears to us that one can present arguments in favor of a positive answer. In fact, as is clear from (44), upon an increase of g by an amount π/L the parameter β increases by π (so long as $g \ll 1$), i.e., the boundary condition at the origin takes its previous form.[9] This can be explained by the above-noted periodicity of the spectrum with respect to the variable g. Since the assignment of β determines the self-adjoint expansion of the Dirac Hamiltonian (which up to this point has only formally been an Hermitian operator), then for arbitrary real values of β the property of completeness must be conserved. Thanks to the Coulomb clustering of the spectrum near $\epsilon = +1$, the total number of levels does not decrease with increasing values of ϵ (in the sense that the cardinal number $\infty - n = \infty$).

The preservation of the completeness properties of the functions serves as an additional argument (even though of a formal order) indicating the consistency of the single-particle description for $\alpha > \alpha_{cr}$.

7. The disappearance of each level into the lower continuum leads to the creation of two positrons.[1] For $L \gg 1$ the values α_{cr} become rather dense and the number of positrons created may be comparatively large.[10] If the bare nucleus Ze created 2n positrons then its charge as $r \to \infty$ would effectively be equal to $Z_{eff} = Z - 2n$ (the reduction of Z_{eff} is due to 2n electrons localized near the nucleus). The following question arises: in what state are these electrons found? A very plausible answer based on physical considerations (due to Ya. B. Zel'dovich) is that the density of this electron cloud is formed out of perturbations of the wave functions in the continuous spectrum (in an energy band $\Delta\epsilon \sim \gamma$ near $\epsilon = \epsilon_0 < -1$, where $\epsilon_0 - i\gamma/2$ denotes the energy of the quasistationary state to which the discrete level has passed after its intersection with the boundary $\epsilon = -1$; see [2]). It would be of interest to verify these qualitative considerations by a more rigorous calculation. The analogous situation in the nonrelativistic case is investigated in article [15].

In conclusion the author wishes to express his sincere gratitude to Ya. B. Zel'dovich and A. B. Migdal for interesting discussions during the course of this work and for a number of valuable comments, and he also thanks V. P. Kraĭnov and A. M. Perelomov for a discussion of the results of this research.

APPENDIX

Certain properties of the Whittaker function $W_{k,\mu}(x)$ are enumerated below. We give special consideration to the case of a purely imaginary index $\mu = ig$, which is most important for the Coulomb problem with $\alpha > 1$, but is not discussed in the existing reference books.[12-14] The function $y = W_{k,ig}(x)$ is real,[11] even with respect to the index g, and satisfies the equation

$$y'' + \left(-\frac{1}{4} + \frac{k}{x} + \frac{g^2 + 1/4}{x^2}\right) y = 0. \quad \text{(A.1)}$$

Its behavior at the ends of the interval $(0, \infty)$ is as follows:

$$W_{k,ig}(x) = a\sqrt{x}\sin(g\ln(1/x) + \delta), \quad x \to 0, \quad \text{(A.2)}$$

$$W_{k,ig}(x) = e^{-x/2}x^k(1 + c_1/x + c_2/x^2 + \ldots), \quad x \to \infty, \quad \text{(A.3)}$$

where

$$ae^{i\delta} = \frac{\Gamma(1+2ig)}{g\Gamma(1/2 - k + ig)}$$

$$c_n = \frac{(-)^n}{n!}[(k - 1/2)^2 + g^2]\ldots[(k - n + 1/2)^2 + g^2].$$

It is not difficult to verify by direct substitution that

$$W_{k,k-1/2}(x) = e^{-x/2}x^k. \quad \text{(A.4)}$$

for any value of k. We also mention the formula

$$W_{k,k+1/2}(x) = e^{-x/2}x^{k+1}\int_0^\infty e^{-xt}(1+t)^{2k}\,dt. \quad \text{(A.5)}$$

One can carry out the numerical calculation of the Whittaker functions according to the formulas[12]

$$W_{k,ig}(x) = \frac{2e^{-x/2}\sqrt{x}}{|\Gamma(1/2 - k + ig)|^2}\int_0^\infty e^{-t}K_{2ig}(2\sqrt{xt})\,t^{-(k+1/2)}\,dt \quad \text{(A.6)}$$

(this relation is valid for $k < 1/2$),

---

[9] If $\beta_1 - \beta_2 = n\pi$, then these two values of β are equivalent since one can always multiply the wave function by a constant (see Eqs. (42)).

[10] Here we wish to correct an error which was made in article [3]. In [3] the critical charge Z_{cr} is called the "electrodynamic boundary of the periodic system of elements," which would be correct if a bare charge with an initial charge $Z > Z_{cr}$ always created $Z - Z_{cr}$ positrons, thereby reducing its effective charge (for an external observer) to the value Z_{cr}. In actual fact the number of positrons created is smaller than $Z - Z_{cr}$. For example, [2] $Z_{cr} = 170$ for $R \sim 10^{-12}$ cm, but the nearest excited level $2P_{1/2}$ reaches the boundary $\epsilon = -1$ for $Z = 185$; therefore, for $170 < Z < 185$ the Coulomb field only creates two positrons. Therefore, in principle electrodynamics does not prohibit the existence of atoms and ions with nuclear charge $Z > Z_{cr}$, but the critical charge is an upper limit only for the existence of bare nuclei which are not surrounded by an electron cloud.

[11] It is understood that the variables k, g, and x have real values, and also $x > 0$.

[12] The usual integral representation (see formula 9.222 in [12]) is not convenient for $\mu = ig$ since it expresses the real function $W_{k,ig}(x)$ in terms of a complex integral.

$$W_{k,ig}(x)=\frac{e^{-x/2}x^{k+\tau}}{\Gamma(\tau)}\int_0^\infty e^{-xt}F(1/2-k+ig,\,1/2-k-ig;\,\tau;\,-t)\,t^{\tau-1}dt \qquad (A.7)$$

(here τ is an arbitrary parameter).

From physical considerations the values $k = \pm 1/2$, 0, corresponding to the energy $\epsilon = 0$ for particles with spin s equal to $1/2$ and 0, have been isolated. In these cases one can expect a simplification of the wave functions. In fact, by selecting $\tau = 1/2$ and $3/2$ in Eq. (A.7) and taking the following equalities into consideration

$$\begin{aligned} F(i\nu,\,-i\nu;\,1/2;\,-\mathrm{sh}^2 x) &= \cos 2\nu x,\\ F(1/2+i\nu,\,1/2-i\nu;\,1/2;\,-\mathrm{sh}^2 x) &= \frac{\cos 2\nu x}{\mathrm{ch}\, x},\\ F(1+i\nu,\,1-i\nu;\,3/2;\,-\mathrm{sh}^2 x) &= \frac{\sin 2\nu x}{\nu\,\mathrm{sh}\, 2x}, \end{aligned} \qquad (A.8)$$

we obtain formulas which are much more convenient for numerical calculations:

$$\begin{aligned} W_{1/2,i\nu}(x) &= \frac{x}{\sqrt{\pi}}\int_0^\infty e^{-\frac{1}{2}x\,\mathrm{ch}\, t}\,\mathrm{ch}\frac{t}{2}\cos\nu t\,dt,\\ W_{-1/2,i\nu}(x) &= \frac{x}{\nu\sqrt{\pi}}\int_0^\infty e^{-\frac{1}{2}x\,\mathrm{ch}\, t}\,\mathrm{sh}\frac{t}{2}\sin\nu t\,dt,\\ W_{0,i\nu}(x) &= \sqrt{\frac{x}{\pi}}\int_0^\infty e^{-\frac{1}{2}x\,\mathrm{ch}\, t}\cos\nu t\,dt = \sqrt{\frac{x}{\pi}}K_{i\nu}\left(\frac{x}{2}\right). \end{aligned} \qquad (A.9)$$

In particular, $\nu = 0$

$$W_{1/2,0}(x) = e^{-x/2}\sqrt{x}, \quad W_{-1/2,0}(x) = e^{x/2}\sqrt{x}\int_x^\infty \frac{e^{-t}}{t}dt, \qquad (A.10)$$

which agrees with Eq. (A.5).

The case $g = 0$ in the Coulomb problem corresponds to $\alpha = |\kappa|$, i.e., it corresponds to the critical value of the coupling constant α for a point charge. In this connection

$$W_{k,0}(x) = e^{-x/2}\sqrt{x}\;\;\Psi(1/2-k,\,1;\,x), \qquad (A.11)$$

where Ψ denotes one of the forms of the degenerate hypergeometric function:[13]

$$\Psi(\varkappa,1;x) = \frac{1}{\Gamma(\varkappa)}\int_0^\infty e^{-xt}t^{\varkappa-1}(1+t)^{-\varkappa}dt. \qquad (A.12)$$

As $x \to 0$ the function $W_{k,0}(x)$ has, in general, a logarithmic singularity. Values of the subscript $k = n + 1/2$ are an exception, when the poles of the Γ-function in Eq. (A.12) cancel this singularity. Then we have

$$W_{n+1/2,0}(x) = (-)^n n!\, e^{-x/2}\sqrt{x}L_n(x), \qquad (A.13)$$

where $L_n(x)$ is the Laguerre polynomial ($n = 0, 1, 2, \ldots$).

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