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90th ANNIVERSARY OF A.B. MIGDAL'S BIRTHDAY
NUCLEI

Critical Charge in Quantum Electrodynamics

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Abstract—The critical nuclear charge Z_{cr} and the critical distance R_{cr} in the system of two colliding heavy nuclei—they are defined as those at which the ground-state level of the electron spectrum descends to the boundary of the lower continuum, with the result that beyond them (that is, for $Z > Z_{cr}$ or $R < R_{cr}$) spontaneous positron production from a vacuum becomes possible—are important parameters in the quantum electrodynamics of ultrastrong Coulomb fields. Various methods for calculating Z_{cr} and R_{cr} are considered, along with the dependence of these quantities on the screening of the Coulomb field of a nucleus by the electron shell of the atom, on an external magnetic field, on the particle mass and spin, and on some other parameters of relevance. The effective-potential method for the Dirac equation and the application of the Wentzel–Kramers–Brillouin method to the Coulomb field for $Z > 137$ and to the two-body Salpeter equation for the quark–antiquark system are discussed. Some technical details in the procedure for calculating the critical distance R_{cr} in the relativistic problem of two Coulomb centers are described. © *2001 MAIK "Nauka/Interperiodica".*

Dedicated to the blessed memory
of Arkadiĭ Benediktovich Migdal
and Mikhail Samuilovich Marinov

Es war … eine Zeit die Riesen brauchte und Riesen zeugte,
Riesen an Denkkraft, Leidenschaft und Character,
an Vielseitigkeit und Gelehrsamkeit.
Friedrich Engels "Dialektik der Natur"[1)]

Mighty, Immense, and Great is the Distant Astral Law …

1. INTRODUCTION

Thirty years ago, there arose interest in the predictions of quantum electrodynamics (QED) in ultrastrong Coulomb fields—in particular, in the effect of spontaneous positron production from a vacuum (see, for example, [1–30] and the review articles [7, 31–39]). A feature peculiar to this process is that it has no bearing on the frequency of an electric field and can occur in the case of an arbitrarily slow (adiabatic) growth of the nuclear charge in the region $Z > Z_{cr}$, a point where it differs from any other positron-production mechanism known so far. Moreover, its probability cannot be computed by perturbation theory,[2)] so that it is necessary to analyze exact solutions to the Dirac equation in an external field.

The problem was formulated by Pomeranchuk and Smorodinsky [40], who considered, as far back as 1945, the energy spectrum of an electron in a Coulomb field with allowance for a finite radius of a nucleus and obtained the first ever estimate for Z_{cr}. After that, however, the problem was not investigated for a long time.

After the year 1969, there appeared a torrent of theoretical studies devoted to this and some other allied problems. Various aspects of spontaneous positron production (as well as of accompanying processes like induced positron production, which is associated with a nonzero frequency of the electric field as the nuclei involved approach; pair conversion in the case of the Coulomb excitation of colliding nuclei; and delta-electron production[3)]) were analyzed in detail both for the case of an isolated superheavy nucleus and for the case where two heavy nuclei such that $Z_1 + Z_2 > Z_{cr}$—for example, uranium nuclei—approach each other. The theoretical description of the structure of the vacuum electron shell of a supercritical ($Z > Z_{cr}$) atom in [7, 15–17] proved to be somewhat out of the ordinary. This range of problems was comprehensively analyzed in the review articles [7, 31–39], where the interested reader can find all necessary details.

[1)]It was ... a time which called for giants and produced giants—giants in power of thought, passion and character, in universality and learning [quoted from Friedrich Engels, *Dialectics of Nature* (Progress Publishers, Moscow, 1982; translated from the German by Clemens Dutt)].

[2)]The probability of spontaneous positron production exhibits a nonanalytic (in the parameter $\zeta = Z\alpha$, α being the fine-structure constant) threshold behavior for $Z \longrightarrow Z_{cr}$ [see Eq. (37) below].

[3)]These accompanying processes must be taken into account in performing relevant experiments. For all these questions, the reader is referred to [7, 10, 21, 25, 39].

The present article, whose objective is less ambitious, is aimed at describing and discussing various methods for calculating the critical nuclear charge Z_{cr} and the critical distance R_{cr} for a collision of two heavy nuclei, as well as at analyzing some equations for the energies of the levels of the electron spectrum in the region $Z \gtrsim Z_{cr}$. The above quantities are basic physical parameters of the problem, which appear in all equations that are used in the theory of spontaneous positron production. At the same time, these questions have not yet received adequate attention in the surveys known to the present author.

In the following, use is made, as a rule, of the system of units where $\hbar = c = m = 1$ (m is the electron mass); distances and ε, the energy of a level, are measured in, respectively, $\hbar/mc = 386.2$ fm and mc^2 units; $\alpha = e^2/\hbar c = 1/137$; and $\zeta = Z\alpha$. The rest energy is included in ε, so that the values of $\varepsilon = 1$ and -1 correspond, respectively, to a free electron at rest (boundary of the upper continuum for solutions to the Dirac equation) and to the boundary of the lower continuum.

This article is dedicated to the memory of Arkadiĭ Benediktovich Migdal (1911–1991) and Mikhail Samuilovich Marinov (1939–2000). Discussions with Arkadiĭ Benediktovich (AB as we called him in a narrow circle of physicists) on various aspects of the QED of strong fields, as well as on a wider range of physical (and not only physical) topics, were always extremely interesting and instructive for me. Recollecting the past, I would like to mention some features that were calling cards of his personality as it remained in my memory. First, it was his desire to understand always the result of any complicated calculations in simple physical terms or on the basis of an appropriate model. Second, it was AB's love for the semiclassical approach, which he knew in minute detail and was able to apply to intricate physics problems (in this connection, see, for example, his remarkable monograph [41]). Third, AB was highly democratic: he would have discussed scientific problems in just the same way with a student and with an academician, while his disapproval of some ideas, which was sometimes expressed very sharply, never became personal (I know this from my own experience). Finally, it was his scientific audacity: for example, AB was not afraid to admit violation of the Pauli exclusion principle for electrons that have descended to the lower continuum [30] and had stubbornly advocated his opinion for quite a long period of time despite the objections and criticism of many Soviet theoretical physicists.[4)] These are the features of AB's scientific style that impressed me most deeply. It would be no wonder to me, however, if such a list as composed by some other contemporary of AB were totally different—is it not true that he was so forceful and diverse a personality that he could be compared (in my opinion) to such creators of the Renaissance period as Geronimo Cardano or Benvenuto Cellini?

I would also like to recollect the discussion on the problem of positron levels that would emerge with increasing Z from the lower continuum. It was in 1970, and it was AB, YaB (Yakov Borisovich Zeldovich), and the present author who participated in this discussion. At that time, AB firmly believed in the existence of such states, while YaB and I questioned this and raised some objections. Our objections annoyed AB, and the discussion became very hot. Finally, Yakov Borisovich said, "Kadya, you have forgotten about the Pauli exclusion principle." The reaction of AB was instantaneous and tempestuous, and everything ended in the following words of Yakov Borisovich: "Kadya, let us finish today at this point, but do not think, please, that I could not answer to you properly and in the same tone, but the presence of Vladimir Stepanovich troubles me somewhat." This scene is still before my eyes, but I do not take courage to go in further details, for this requires greater writing abilities. This episode was reflected in part in the article written by Zeldovich and the present author [7].

Many years of friendship and cooperation connected me with Misha Marinov (some results of our joint work—in particular, those concerning spontaneous positron production—were used in the present article, especially in Section 3), who was a highly educated physicist and who possessed a deep knowledge of mathematics and a great pedagogical talent. I recall with admiration lectures (brilliant in form and excellent in content) on exceptional Lie groups, Cayley octanions, and Grassmann numbers that Misha delivered at the Institute of Theoretical and Experimental Physics (Moscow) shortly after these mathematical constructions (nearly unknown to theoretical physicists at that time) had come into use in the theory of elementary particles.

2. CRITICAL CHARGE OF A NUCLEUS

The discrete spectrum of the energy levels of an electron moving in the Coulomb field of a nucleus falls within the range $-1 \le \varepsilon < 1$. The problem admits an analytic solution in the case of a pointlike charge, where the energy levels are determined by the well-known Sommerfeld fine-structure formula [42]. For example, the energy of the $1s_{1/2}$ ground-state term in the Coulomb field $V(r) = -\zeta/r$ is given by

$$\varepsilon_0(\zeta) = \sqrt{1-\zeta^2}, \quad 0 < \zeta = Z\alpha < 1. \qquad (1)$$

The curve of the $1s$ level terminates at $Z = \alpha^{-1} = 137$ and $\varepsilon_0 = 0$, not reaching the boundary of the lower contin-

[4)] Of course, AB was wrong in this case, but this example is a good illustration of a feature that was peculiar to his personality—the total absence of reverence for commonly recognized authorities.

uum. For the energy-degenerate $ns_{1/2}$ and $np_{1/2}$ states for $\zeta \longrightarrow 1$, we similarly have

$$\varepsilon_n(\zeta) = \frac{n-1}{N_0} + \frac{1}{N_0^3}\sqrt{1-\zeta^2} + O(1-\zeta^2), \qquad N_0 = \sqrt{n^2 - 2n + 2}, \tag{1a}$$

where $n = 0, 1, 2, \ldots$ is the principal quantum number. A formal analytic continuation of $\varepsilon_n(\zeta)$ to the region $Z > 137$ leads to imaginary values of energy and complex-valued wave functions, but this is unsatisfactory from the physical point of view.[5)] The reason behind the emergence of this difficulty can easily be traced with the aid of the effective-potential method [4, 7, 18].

For the sake of simplicity, we begin by considering the case of spherical symmetry, $V = V(r)$. Upon a separation of the variables, the Dirac equation in a central field reduces to a set of differential equations for the radial wave functions $g(r)$ and $f(r)$. The substitution

$$\varphi = W^{-1/2}g, \quad W = 1 + \varepsilon - V(r), \tag{2}$$

where g corresponds to the upper component of the Dirac bispinor [45], recasts these equations into a form similar to the Schrödinger equation but with an effective energy E and an effective potential U. Specifically, we have

$$E = (\varepsilon^2 - 1)/2,$$
$$U(r) = \varepsilon V - \frac{1}{2}V^2 + \frac{\kappa(\kappa+1)}{2r^2} + \frac{V''}{4W} + \frac{3}{8}\left(\frac{V'}{W}\right)^2 - \frac{\kappa V'}{2rW}, \tag{3}$$

where the quantum number $\kappa = \mp(j + 1/2)$ corresponds to $j = l \pm 1/2$ states, j and l being, respectively, the total angular momentum of the electron and its orbital angular momentum (for the upper component g). We note that the effective potential U depends on the angular momentum j and on the energy ε of a level and that it takes markedly different forms for ε values close to +1 and –1. For the Coulomb field of a pointlike nucleus, we have

$$U(r) = \begin{cases} \dfrac{j(j+1)-\zeta^2}{2r^2} + \ldots & \text{for} \quad r \longrightarrow 0 \\ -\dfrac{\varepsilon\zeta}{r} + \dfrac{\kappa^2 - \zeta^2 + a}{2r^2} + \ldots & \text{for} \quad r \longrightarrow \infty \end{cases} \tag{4}$$

($a = \kappa$ for $\varepsilon > 1$ and $a = -1/4$ for $\varepsilon = -1$).

At sufficiently large values of the charge Z, a singular attraction that is in inverse proportion to the radius squared and which can lead to collapse into the center [46–49] (a phenomenon well known in quantum mechanics) arises in the effective potential at small distances. In order to demonstrate this, we consider a trial function different from zero only in the region $0 < r < r_0$. In accordance with the Heisenberg uncertainty relation, one has $\langle p^2\rangle r_0^2 \geq 1/4$, whence it follows that

$$\langle H\rangle = \frac{1}{2}\langle p^2\rangle + \langle U\rangle \leq \frac{(j+1/2)^2 - \zeta^2}{2r_0^2} + O\left(\frac{1}{r_0}\right),$$
$$r_0 \ll 1.$$

For $\zeta > j + 1/2$, the spectrum of the effective Hamiltonian H is not bounded from below, since we have $\langle H\rangle \longrightarrow -\infty$ for $r_0 \longrightarrow 0$. Such a situation corresponds to collapse into the center of forces in classical mechanics and to the emergence of complex eigenvalues in the case of the Dirac equation, but this is precisely what occurs in the latter case [as can be seen from Eqs. (1) and (1a)] upon a formal continuation of the energy spectrum of levels for a pointlike charge to the region $\zeta > 1$.

From the aforesaid, it is clear that the emergence of a singularity in the formulas for $\varepsilon_n(\zeta)$ at $\zeta = 1$ is due to the use of the idealized case of a pointlike charge. This approximation provides a high precision for light nuclei, but it becomes inapplicable at $\zeta > 1$ for the $j = 1/2$ states and at $\zeta > j + 1/2$ for states characterized by the angular momentum j. At such large values of Z, the Dirac equation must be solved with a potential cut off at small distances, whereby the finiteness of nuclear sizes is taken into account. In such a potential,

$$V(r) = \begin{cases} -\zeta/r & \text{for} \quad r > r_N \\ -\dfrac{\zeta}{r_N} f\left(\dfrac{r}{r_N}\right) & \text{for} \quad 0 < r < r_N, \end{cases} \tag{5}$$

the form of the cutoff function $f(r/r_N)$ is dictated by the electric-charge distribution over the nuclear volume (see Appendix A).

Pomeranchuk and Smorodinsky [40] were the first to notice this. By introducing finite nuclear sizes, they showed that the Dirac equation has a solution over the entire region from $Z = 0$, $\varepsilon = 1$ to $Z = Z_{cr}$, $\varepsilon = -1$ and roughly estimated the critical charge Z_{cr} (however, their estimate proved to be exaggerated). More precise values of Z_{cr} were obtained later in [50, 51]. However, it remained unclear what actually occurs at $Z > Z_{cr}$. For more than 25 years, this problem had not attracted much attention.

A breakthrough occurred in the years 1969 and 1970, when the problem of the critical charge of a nucleus and physical phenomena in the region $Z > Z_{cr}$ became the subject of intensive investigations. First of all, the value of Z_{cr} was calculated precisely for a spherical nucleus. These precise values were obtained independently by two methods. Pieper and Greiner [2] determined the energies of the levels by numerically solving the Dirac equation and found Z_{cr} as the point of intersection of the curve representing the level $\varepsilon_0(\zeta)$ and

[5)] Nonetheless, such a possibility was considered in the literature [43, 44]. There, complex values arise from the absorption boundary condition imposed for $r \longrightarrow 0$.

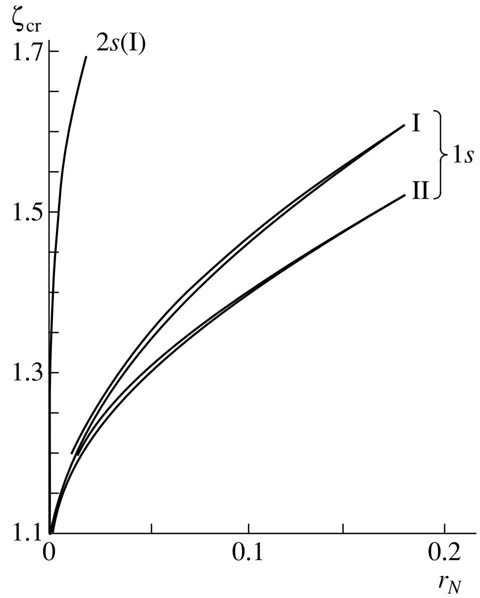

Fig. 1. Critical charge of a nucleus ($\zeta_{cr} = Z_{cr}/137$) for the $1s_{1/2}$ and $2s_{1/2}$ levels (the nuclear radius r_N is given in $\hbar/mc$ = 386 fm units). The cutoff models I and II correspond to the uniform charge distributions over the nuclear surface and volume, respectively. In each pair of close curves, the upper and the lower one represent, respectively, the results of the numerical calculation from [3] and the results obtained with the semiclassical formula (45).

the boundary of the lower continuum (they assumed that the nuclear charge is uniformly distributed over the volume of a sphere of radius $r_N = r_0A^{1/3}$, where r_0 = 1.2 fm and where the dependence of the atomic number A on the nuclear charge was approximated by the formula $A = 63.6 + 1.30Z + 0.00733Z^2$, which was obtained from a dedicated consideration for a region of superheavy nuclei ($100 < Z < 250$).

On the other hand, it was noticed in [3] that solutions to the Dirac equation are strongly simplified at $\varepsilon = -1$. Owing to this, it is possible to derive an equation immediately for Z_{cr}. The result is

$$zK'_{i\nu}(z)/K_{i\nu}(z) = 2\xi, \tag{6}$$

where $z = \sqrt{8\zeta_{cr}r_N}$, $\nu = 2\sqrt{\zeta_{cr}^2 - \kappa^2}$, $K_{i\nu}(z)$ is a Macdonald function,[6)] and $\xi = \xi(\zeta, \kappa)$ is the logarithmic derivative of the intrinsic wave function at the nuclear boundary [see Eq. (A.2) in Appendix A]. A numerical solution to Eq. (6) was constructed for the case of $r_N = r_0A^{1/3}$ with r_0 = 1.1 fm and $A = 2.6Z$ (these values are typical of heavy nuclei) and for the following two cutoff models:

$$\left.\begin{aligned} &\mathrm{I} \quad f(x) \equiv 1 \\ &\mathrm{II} \quad f(x) = (3 - x^2)/2 \end{aligned}\right\} \quad \text{for} \quad 0 < x \equiv r/r_N < 1.$$

[6)] It is a real-valued function at real ν and $z > 0$, which decreases in proportion to $\exp(-z)$ for $z \longrightarrow \infty$ and which features an infinite number of oscillations for $z \longrightarrow 0$.

Of these, the second corresponds to a constant density of the electric charge in a nucleus. For a few low-lying levels, the results of the calculations based on model II are the following:

$$Z_{cr} = 169(1s_{1/2}), \quad 185(2p_{1/2}), \quad 230(2s_{1/2}), \ldots \tag{7}$$

(see also Fig. 1). These values are in good agreement with those from [2].

In this connection, there arises the problem of sensitivity of Z_{cr} values to a detailed form of the nuclear-density distribution in superheavy nuclei. This problem can be resolved by comparing the Z_{cr} values as obtained for the cutoff models I and II—the point is that model I assumes that the charge is entirely concentrated on the nuclear surface, while model II corresponds to a uniform electric-charge distribution over the nuclear volume and is therefore quite realistic. Upon going over from model I to model II, the value of the electrostatic potential at the center of a nucleus increases by a factor of 1.5, amounting to $V(0) = 1.5\zeta/r_N \simeq 70mc^2$ = 35 MeV. The corresponding values of ζ_{cr} at r_N = 10 fm are Z_{cr} = 1.271 (I) and 1.243 (II), the difference of Z_{cr} values within models I and II being 3.8 units. From these results alone, we can conclude that less significant modifications (like allowances for the diffuseness of the nuclear boundary, for deviations from a spherical shape of nuclei, and for changes in the relationship between A and Z in superheavy nuclei) would lead to very modest modifications (of not more than one unit) to Z_{cr} (these effects were estimated in [13, 18, 25]). For the critical charge Z_{cr} of a naked nucleus (that is, a nucleus not surrounded by an electron shell), we can take the values in (7).

So far, the nucleus has been considered to be naked—that is, completely deprived of its electron shell. But if it is surrounded by such a shell, the shell electrons reside near the nucleus for some part of the time, screening its charge; as a result, Z effectively becomes smaller, so that Z_{cr} increases. Estimating this effect is especially important in connection with performing experiments to study spontaneous positron production in heavy-ion collisions. Indeed, the total charge of nuclei, $Z_1 + Z_2$, can exceed the critical charge $Z_{cr} \approx 170$ calculated without allowing for screening only by 15–20 units; therefore, an increase in Z_{cr} even by 10 units would considerably complicate an experiment with heavy nuclei available at present.

Since it is very difficult to calculate Z_{cr} in the problem of two centers, the analysis was actually performed for a spherical nucleus. The electron-shell density was taken according to the Thomas–Fermi equation [52]. Although the speed of K-shell electrons is $v \sim c$, the majority of electrons occur at distances of $r \sim 137Z^{-1/3} \gg 1$ from the nucleus, so that the use of the nonrelativistic Thomas–Fermi model is justified. For the screening-induced increase in the critical charge, the results obtained in [11] and [19] for the case of a neutral atom are ΔZ_{cr} = 1.5 and 1.2, respectively. A modest distinction between these two values seems to be due to the use of the different shapes of the electron-charge distribution within the nucleus in those studies. Moreover, the screening of the nuclear charge was taken into account more correctly in [11] on the basis of the relativistic Hartree–Fock–Slater equation (see [12]), and the value of $Z_{cr} = 173$ was obtained there. Summing the different corrections, we find that, upon a transition from the cutoff model II to a nucleus that has a diffuse boundary and which is surrounded by an electron shell, the Z_{cr} values presented in (7) increase by approximately 3 ± 1 units for the 1*s* and 2*p* states (see Table 1). It is also possible to investigate Z_{cr} as a function of the degree of ionization of the electron shell, $q = (Z - N)/Z$, where N is the total number of electrons in the shell (we have $q = 0$ for a neutral atom and $q = 1$ for a naked nucleus). With allowance for the screening effect, the self-consistent potential for an electron now becomes

$$V_q(r) = -\left(\frac{Z}{r_N} f(r/r_N) + \frac{Z-N}{r_0}\right) e^2 \text{ for } 0 < r < r_N;$$

$$V_q(r) = -\left(\frac{Z}{r} \varphi(x) + \frac{Z-N}{r_0}\right) e^2 \text{ in the region } r_N < r < r_0;$$

and

$$V_q(r) = -(Z-N)e^2/r$$

for $r > r_0$, where $\varphi(x)$ is a solution to the Thomas–Fermi equation for an ion, $x = (128Z/9\pi^2)^{1/3} r/a_B = 0.0425\zeta^{1/3} r$, and r_0 is the radius of a positive ion in the Thomas–Fermi model [52] [here, $r_0 \longrightarrow \infty$ at $q = 0$ ($r_0 \gg r_N$)].

A change in Z_{cr} can be found by perturbation theory [18]. Specifically, we have

$$\delta\zeta_{cr} = \beta^{-1}\langle\delta V\rangle, \quad \langle\delta V\rangle = \int \delta V(r)\rho_{cr}(r) r^2 dr, \quad (8)$$

where $\rho_{cr} = \psi^+\psi$ is the electron-shell density at the critical point and β is the slope of the level [see Eq. (12) below]. Substituting the expression $\delta V = V_q(r) - V_0(r)$ into (8) and considering that the main contribution to the relevant integral comes from the region where $r \sim r_K \ll r_a$ (r_K is the *K*-shell radius, and r_a is the mean radius of the atom), we obtain [53]

$$\Delta Z_{cr}(q) = \Delta Z_{cr}(0) F(q). \quad (9)$$

The correction $\Delta Z_{cr}(0)$ for a neutral atom was found by numerically solving the Dirac equation for $\varepsilon = -1$ and $V(r) = -\zeta r^{-1}\varphi_0(x)$. The results of the calculation are quoted in Table 1; the graph of the function $F(q)$ is depicted in Fig. 2, where we can see that, in the region $q \lesssim 0.5$, this function changes insignificantly—for example, $F(0.5) = 0.907$ [q values around 0.5 correspond to a (Z_1, Z_2, e) quasimolecule arising in a collision of a naked nucleus with a neutral atom, because we usually have $Z_1 \approx Z_2$)]. Thus, the correction for screening in an ion whose degree of ionization is $q \sim 0.5$ is nearly identical to that in a neutral atom. This can easily be understood: with increasing degree q of ionization, the electron shell comes closer to the nucleus, whereby a decrease in the screening shell charge, which is equal to $(1 - q)Z$, is partly compensated. On the other hand, the correction ΔZ_{cr} decreases fast when we go over to a naked nucleus ($q \longrightarrow 1$) since $F(q) \propto (1-q)^{1/3} \longrightarrow 0$.

Table 1. Critical charge for a spherical nucleus (lowest states with $\kappa = \mp 1$)

	$1s_{1/2}$	$2p_{1/2}$	$2s_{1/2}$	$3p_{1/2}$
$Z_{cr}^{(0)}$	168.8	181.3	232	254
ΔZ_{cr}	1.2	1.1	3.5	3.3
$\Delta Z_{cr}'$	0	1.5	3.1	4.6
$\Delta Z_{cr}''$	0.5	0.6	0.8	1.0
Z_{cr}	170.5	184.5	239	263
ζ_{cr}	1.245	1.346	1.74	1.92
$\langle r\rangle$	0.500	1.27	2.27	5.76
	0.309	0.237	0.552	0.459
$\rho(\zeta = \zeta_{cr})$	1.62	0.333	0.994	0.333

Note: The following notation is used here: $Z_{cr}^{(0)}$ is the critical charge for a naked nucleus with a sharp boundary (cutoff model II); ΔZ_{cr} is the correction for screening in a neutral atom; $\Delta Z_{cr}'$ is the correction for screening by the vacuum shell; $\Delta Z_{cr}''$ is the correction due to the diffuseness of the nuclear boundary; and $\langle r\rangle$ is the mean radius of the electron state in $\hbar/mc$ units: (first row) at $\zeta_{cr}^{(0)} = 1$ (for a pointlike nucleus) and (second row) at $\zeta = \zeta_{cr}$ with allowance for finite nuclear sizes. The parameter ρ is defined in (31) and (B.13).

The calculations presented in [53] also took into account the screening of the nuclear charge by a vacuum shell of a supercritical atom (whose $Z > Z_{cr}$ nucleus attracts such a shell upon positron emission [26, 54]) and the diffuseness of the nuclear boundary. The eventual results of those calculations for Z_{cr} are given in Table 1.

It is interesting to find out how finite nuclear sizes eliminate the singularity of the energy $\varepsilon_0(\zeta)$ at $\zeta = Z\alpha = 1$. Suppose that the cutoff radius r_N is arbitrarily small in relation to the electron Compton wavelength. In the limit $\Lambda = \ln(1/r_N) \gg 1$ (which is of a somewhat academic interest), the energy of the 1*s* level becomes [5, 7]

$$\varepsilon_0(\zeta) = \gamma \coth \Lambda\gamma, \quad \gamma = \sqrt{1-\zeta^2}. \quad (10)$$

In the region $Z < 137$, $\coth\Lambda\gamma = 1 + \exp(-2\Lambda\gamma) + \ldots$ tends to unity exponentially fast, so that, for $1 - \zeta \gg \Lambda^{-2}$, the energy $\varepsilon_0(\zeta)$ coincides with expression (1) for a pointlike charge and is virtually independent of the way in which the Coulomb potential is cut off within the nucleus. On the other hand, the point $\zeta = 1$ is no longer a singular point for the function $\varepsilon_0(\zeta)$ at $r_N > 0$, and

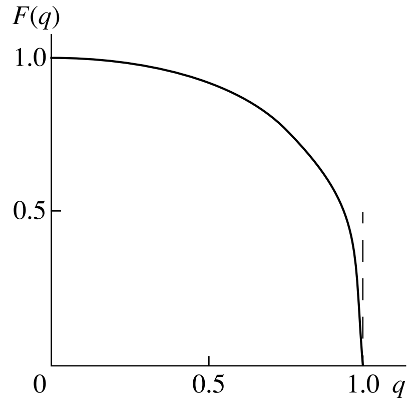

Fig. 2. Graph of the function $F(q)$ in (9) ($q = 1 - N/Z$ is the degree of ionization of the electron shell of a superheavy atom).

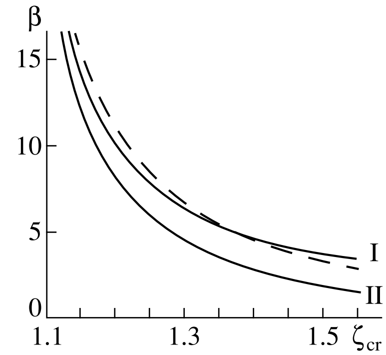

Fig. 3. Slope β of the ground-state level entering the lower continuum: (solid curves) results of the numerical calculation from [4] and (dashed curve) result obtained in the semiclassical approximation [74] for the cutoff model I.

expression (10) can be continued to the region $Z > 137$ with the result

$$\varepsilon_0(\zeta) = \tilde{\gamma}\coth\Lambda\tilde{\gamma}, \quad \tilde{\gamma} = \sqrt{\zeta^2 - 1}. \tag{10a}$$

Expressions (10) and (10a) describe a unified analytic function that, in the vicinity of the point $\zeta = 1$, is expanded in a convergent series in integral powers of $1 - \zeta^2$ as

$$\varepsilon_0(\zeta) = \frac{1}{\Lambda}\left\{1 + \sum_{n=1}^{\infty} 2^{2n}\frac{B_{2n}}{(2n)!}\Lambda^{2n}(1-\zeta^2)^n\right\}, \tag{10b}$$

where B_{2n} are Bernoulli numbers [$B_2 = 1/6$, $B_4 \equiv -1/30$, $\ldots$, $B_{2n}/(2n)! \approx 2(-1)^{n-1}(2\pi)^{-2n}$ for $n \longrightarrow \infty$]. Expression (10a) has a pole at $\tilde{\gamma} = \pi/\Lambda$,[7)] whence we obtain the asymptotic formula

$$\zeta_{cr} = 1 + \frac{\pi^2}{2\Lambda^2} + O(\Lambda^{-3}), \quad \Lambda \gg 1. \tag{11}$$

We can see from this formula that ζ_{cr} as a function of the cutoff radius r_N has a singularity for $r_N \longrightarrow 0$. Therefore, finite nuclear sizes cannot be taken into account by perturbation theory if $Z > 137$. Here, collapse into the center for the Dirac equation with a pointlike Coulomb potential clearly manifests itself.

In the zero-range limit ($r_N = 0$), the curve representing the 1*s* level reaches the point $\varepsilon = 0$ at $\zeta = 1$ and steeply terminates after that (the derivative is $d\varepsilon_0/d\zeta = -\infty$). This shows that the zero-range approximation is inapplicable to the problem being considered. At the same time, the function $\varepsilon_0(\zeta)$ smoothly intersects the line $\varepsilon = 0$ if $r_N > 0$, showing no singularities there, and enters the lower continuum with a finite slope β:

$$\beta = -\frac{d\varepsilon}{d\zeta}\bigg|_{\zeta = \zeta_{cr}} = \int v(\mathbf{r})\rho_{cr} d^3 r, \qquad \rho_{cr} = \psi_0^2(r)|_{\zeta = \zeta_{cr}} \tag{12}$$

(Fig. 3). Here, we have written the potential in the form $V(\mathbf{r}) = -\zeta v(\mathbf{r})$, assuming that the function v determining the shape of the potential no longer depends on ζ [for the potential in Eq. (5), this holds to a high precision, since the dependence $r_N \propto \zeta^{1/3}$ is rather weak]. The parameter β determines the threshold behavior of the probability of spontaneous positron production [4, 21].

The properties of atomic states for $Z > 137$ were also investigated. Presented below are the formulas for the mean radius of the ground state and for its variance. For a $Z < 137$ pointlike nucleus, we have [see Eqs. (B.2) and (B.9)]

$$\langle r\rangle = (1 + 2\sqrt{1-\zeta^2})/2\zeta, \quad \Delta r = \frac{\langle r\rangle}{(1 + 2\sqrt{1-\zeta^2})^{1/2}}. \tag{13}$$

For the $\kappa = -1$ states (that is, $ns_{1/2}$ states), the results at the boundary of the lower continuum are

$$\langle r\rangle = \frac{(4\zeta_{cr}^2 - 3)(1 + 0.3\zeta_{cr}^2)}{2\zeta_{cr}(2\zeta_{cr}^2 + 3)}, \quad \varepsilon = -1 \tag{14}$$

(see Table 1). For an arbitrary energy of a level, $0 > \varepsilon > -1$, the expression for $\langle r\rangle$ is much more complicated [3]. According to numerical calculations, the mean radius of the ground state decreases monotonically with increasing ζ (see Fig. 5 in [3]), this decrease being especially pronounced when the charge increases from $Z = 137$ to Z_{cr} (compare the corresponding numbers in Table 1); on the contrary, the relative variance $\Delta r/\langle r\rangle$

7) In fact, this pole is spurious—it is removed in solving the problem more accurately, whereby it is shown that, near the critical point, there is a comparatively narrow region $\zeta_{cr} - \zeta \sim \Lambda^{-3}$, where expression (10a) is inapplicable. The relevant expression for the energy of the level can be found in [5].

increases. The magnetic moment of the electron in a bound state is given by [6]

$$\mu_{cr} \equiv \mu(\zeta = \zeta_{cr}) = 2(4\zeta_{cr}^2 - 3)/3(2\zeta_{cr}^2 + 3), \quad \kappa = -1. \tag{15}$$

In particular, $\mu_{cr} \longrightarrow 2/15 = 0.133$ for $\zeta_{cr} \longrightarrow 1$ and $\mu_{cr} = 0.350 \approx 1/3$ of the Bohr magneton for $\zeta_{cr} = 1.245$ (1*s* ground state).

Equations (13)–(15) can easily be generalized to other states of the discrete spectrum (see Appendix B). Table 1 also quotes the values of the parameter $\rho = w_2/w_1$, which characterizes the relative weight of the lower and the upper component of the Dirac bispinor [see Eq. (B.13)]. Since $\rho \sim 1$, the electron bound state at the boundary of the lower continuum is fully relativistic (as might have been expected).

Equations (6), (14), and (15) have so simple a form owing to the fact that, in the case of the Coulomb field $V(r) = -\zeta/r$, solutions to the Dirac equation at $\varepsilon = -1$ that decrease at infinity are explicitly expressed in terms of a Macdonald function as

$$\begin{aligned} G(r) &\equiv rg(r) = K_{i\nu}(z), \\ F(r) &\equiv rf(r) = \zeta^{-1}(rG' + \kappa G) \\ &= \zeta^{-1}\left[\kappa K_{i\nu}(z) + \frac{1}{2} z K'_{i\nu}(z)\right] \end{aligned} \tag{16}$$

(the normalization factors are omitted here), where $z = 2^{3/2}(\zeta r)^{1/2}$, $\nu = 2(\zeta^2 - \kappa^2)^{1/2}$, $\zeta > |\kappa|$, and the radial wave functions $g(r)$ and $f(r)$ correspond to the definition given in [45], the normalization condition being $\int_0^\infty (G^2 + F^2)dr = 1$ here (in the limit $r_N \longrightarrow 0$, the normalization factor can be calculated explicitly [4, 21]). From (16), it follows that, in the limit $r \longrightarrow \infty$, we have

$$\begin{aligned} G(r) &\approx c_1 r^{-1/4} \exp(-\sqrt{8\zeta_{cr} r}), \\ F(r) &\approx c_2 r^{1/4} \exp(-\sqrt{8\zeta_{cr} r}), \end{aligned} \tag{17}$$

the ratio of the coefficients c_1 and c_2 being $c_1/c_2 = -\sqrt{\zeta_{cr}/2}$. Thus, the electron level that reached the boundary of the lower continuum remains localized (compare with the results given in [1]). At large distances from the nucleus, we then have $F/G \propto \sqrt{\zeta r} \gg 1$ and the electron-shell density decreases exponentially,

$$\begin{aligned} \rho_{cr}(r) &= (G^2(r) + F^2(r))/4\pi r^2 \\ &\approx \text{const} \times r^{-3/2} \exp(-c_3\sqrt{\zeta_{cr} r}), \quad r \longrightarrow \infty, \end{aligned} \tag{17a}$$

with the numerically large coefficient of $c_3 = 2^{5/2} = 5.657$.

A considerable simplification in Eqs. (14)–(16) in relation to the general case of $\varepsilon \neq -1$ may be due to some additional symmetry of the Dirac equation. In this connection, it should be noted that the group of the hidden symmetry of the hydrogen atom (for the nonrelativistic case, it was discovered by Fock [55] and Bargmann [56]; see also [57–62]) was considered in [63–65] for the relativistic Coulomb problem. However, no special analysis has been performed for $\varepsilon = -1$ states at the boundary of the lower continuum.

3. CRITICAL DISTANCE FOR COLLIDING NUCLEI

There are no nuclei with charge $Z \sim Z_{cr} > 170$ in nature, and prospects for synthesizing them are absolutely unclear at present.[8] It was noted by Gershtein and Zeldovich [1], however, that supercritical electric fields are generated for a short period of time in the case where two ordinary heavy ions (for example two naked uranium nuclei with total charge $Z_1 + Z_2 = 184 > Z_{cr}$) come to each other within a distance R less than the critical distance R_{cr}. Such an experiment is quite feasible, and the corresponding theoretical problem is that of two centers for the Dirac equation. Since the nuclei involved move at nonrelativistic velocities ($v_N/c \approx 1/20$) and since a K electron is relativistic for $Z\alpha \gtrsim 1$, the energies of the electron terms can be calculated in the adiabatic approximation. The charge of each of the colliding nuclei is less than 137, whence it follows that finite nuclear sizes can be taken into account by perturbation theory. Solving the Dirac equation for two pointlike charges at rest that occur at a distance R from each other and which generate the potential

$$V(\mathbf{r}) = -\left(\frac{Z_1\alpha}{r_1} + \frac{Z_2\alpha}{r_2}\right), \quad r_{1,2} = |\mathbf{r} \pm \mathbf{R}/2|, \tag{18}$$

where $r_{1,2}$ are the distances between the electron and the nuclei involved, presents the most serious difficulty in the problem. This problem is much more complicated than the above problem of solving the Dirac equation for a spherical nucleus.

The Schrödinger equation with the potential (18) has received a comprehensive study [67] (it has numerous applications in the theory of molecules, in the physics of muon catalysis, and in some other allied realms). In this case, variables in the nonrelativistic Schrödinger equation are separated in the ellipsoidal coordinates (see [48])[9]

$$\xi = \frac{r_1 + r_2}{R}, \quad \eta = \frac{r_1 - r_2}{R},$$
$$\xi \geq 1, \quad -1 \leq \eta \leq 1, \quad 0 \leq \varphi \leq 2\pi,$$

[8] In this connection, mention should be made of the last record in these realms—the formation of $Z = 114$ and $Z = 116$ nuclei in $^{48}Ca + {}^{242,244}Pu$ interactions (in all, seven such nuclei have been observed so far). In all probability, these nuclear species lie near the island of stability of superheavy elements—its existence has long since been predicted by theorists (see, for example, [66]). Naturally, this also quickens interest in QED predictions in the region $Z > 137$.

[9] In the mathematical literature [47, 67], they are more often referred to as prolate spheroidal coordinates.

and the equation reduces to two ordinary differential equations. In going over to the relativistic problem of two Coulomb centers, we run into the following additional difficulties:

(i) Variables are not separated in any of the known systems of orthogonal coordinates.

(ii) Near each of the nuclei, the wave function develops a singularity associated with the term $-(1/2)V^2$ in the effective potential.

(iii) There is a significant spin–orbit interaction, because of which the upper and the lower spinor component of the wave function are on the same order of magnitude at $Z\alpha \sim 1$.

Squaring the Dirac equation at $\varepsilon = -1$, we arrive at the set of equations

$$\begin{aligned} \Delta\psi_1 + U_{11}\psi_1 + U_{12}\psi_2 &= 0, \\ \Delta\psi_2 + U_{21}\psi_1 + U_{22}\psi_2 &= 0, \end{aligned} \tag{19}$$

where the matrix elements U_{ij} depend on r_1 and r_2 and on the parameters R and ζ (see Appendix C). Upon separating the azimuthal angle φ, we obtain a set of second-order partial differential equations on a plane. A direct application of standard finite-difference methods for solving boundary-value problems for elliptic equations to this set is inappropriate because of the presence of singularities. The critical distance R_{cr} was calculated by the Ritz method [14, 27] or by the Kantorovich method (see [22, 23]).[10)] Either method relies on the variational principle. Within the Ritz method, the ψ function is represented as a finite sum $\psi = \sum_n c_n\varphi_n$, where $\{\varphi_n\}$ is a fixed set of basis functions, while c_n are variable constants. Within the Kantorovich method, $\psi = \sum_n d_n(y)\varphi_n(x)$, where d_n are fixed functions of the variable y, while φ_n are variable functions of x. Substituting the ψ function into the quadratic energy functional, one arrives at a bilinear form in the coefficients c_n within the Ritz method or at a functional bilinear in φ_n within the Kantorovich method.

The condition requiring that the energy be minimal leads to a set of linear algebraic equations within the first method or a set of ordinary differential equations for the functions $\varphi_n(x)$ within the second method. In order to achieve a high precision in variational calculations, it is important to choose correctly the variables x and y and the functions $d_n(y)$; in the Ritz method, success depends on the choice of basis functions φ_n.

The following approach was adopted in [22, 23]. We denote by $\rho = \sqrt{x^2 + y^2}$, z, and φ cylindrical coordinates. If the charges of the nuclei are identical, $Z_1 = Z_2 = Z/2$, the wave function of the ground-state term is symmetric under the inversion in the $z = 0$ plane. In addition, we note that, for the ground-state term, the projection of the total angular momentum of the relevant quasimolecule is $J_z = \Lambda + s_z = 1/2$, while the projection of the orbital angular momentum Λ is zero for ψ_1 and unity for ψ_2. Isolating kinematical factors, we can represent the spinor components as

$$\psi_1(\mathbf{r}) = \chi_1(\rho, z), \quad \psi_2(\mathbf{r}) = \frac{\rho z}{R^2}e^{i\varphi}\chi_2(\rho, z), \tag{20}$$

where χ_1 and χ_2 are real-valued functions that are even in z. Instead of ρ and z, we now introduce the variables $x = x(\rho, z)$ and $y = y(\rho, z)$ in such a way that the singular points of Eqs. (19) occur at $x = 0$ and ∞, irrespective of y. For this, it is sufficient that $x \longrightarrow 0$ when $r_1 \longrightarrow 0$ or $r_2 \longrightarrow 0$ and $x \longrightarrow \infty$ when $r_{1,2} \longrightarrow \infty$. The choice of the variable y is not very important—it is only necessary that the variables x and y be independent. Specifically, use was made of the variables

$$x = \xi^2 - \eta^2 = \frac{r_1 r_2}{4R^2}, \quad y = \frac{\eta^2}{\xi^2 - \eta^2} = \frac{(r_1 - r_2)^2}{4r_1 r_2}, \tag{21}$$

which take values in the curvilinear triangle $(x^{-1} - 1)\theta(1 - x) < y < x^{-1}$ on the (x, y) plane. In terms of these variables, we have $V(\mathbf{r}) = -2\zeta R^{-1}\sqrt{(1 + y)/x}$. The trial functions were represented as

$$\chi_1 = \sum_{k=1}^{m}\varphi_k(x)y^{k-1}, \quad \chi_2 = \sum_{k=1}^{n}\varphi_{m+k}(x)y^{k-1}. \tag{22}$$

A minimization of the energy functional leads to the set of $N = m + n$ equations

$$\frac{d}{dx}\left(P\frac{d\varphi}{dx} + R\varphi\right) - Q\varphi - R^T\frac{d\varphi}{dx} = 0, \qquad \varphi = \begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \vdots \\ \varphi_N \end{pmatrix}, \tag{23}$$

where P, Q, and R are $(N \times N)$ matrices dependent on x. All the coefficients P_{ij}, $Q_{ij}(x)$, and $R_{ij}(x)$ are expressed in terms of elementary functions; by way of example, we indicate that, at $i = j = 1$,

$$P_{11}(x) = x\begin{cases} \sqrt{1+x} - \sqrt{1-x} - \ln\dfrac{1+\sqrt{1+x}}{1+\sqrt{1-x}} & \text{for} \\ 0 < x \le 1 \\ \sqrt{1+x} - \ln[(1+\sqrt{1+x})/\sqrt{x}] & \text{for} \\ x > 1. \end{cases} \tag{24}$$

[10)] The idea of reducing a partial differential equation to a set of ordinary differential equations is due to Kantorovich. Solutions to Poisson's and the biharmonic equation were considered in [68] in various regions on a plane, and it was shown there that, as a rule, this method converges faster than the variational Ritz method and is more accurate than it.

The functions P_{ij}, Q_{ij}, and R_{ij} are continuous at the point $x = 1$, together with their first derivatives;[11] it is convenient to calculate them with the aid of the recursion relations from [22]. The boundary conditions for the functions $\varphi_i(x)$ for $x \longrightarrow 0, \infty$ follow from the requirement that the norm of the ψ function be convergent.

The boundary-value problem specified by Eq. (23) has a solution only at specific $R = R_{cr}(Z)$. The functions $\varphi_k(x)$ have a power-law singularity for $x \longrightarrow 0$ and an essential singularity for $x \longrightarrow \infty$. The character of these singularities and the expansions near them immediately follow from Eqs. (23). Introducing the matrix of logarithmic derivatives,

$$Y = \|Y_{ij}(x)\|, \quad \varphi_i' = \sum_{j=1}^{N} Y_{ij}\varphi_j,$$

we reduce the set of Eqs. (23) to the matrix Riccati equation

$$Y' = A - BY - Y^2, \qquad (25)$$

where

$$A = P^{-1}(Q - R'), \quad B = P^{-1}(R - R^T + P'). \qquad (25a)$$

By numerically solving this equation by the Runge–Kutta method in the intervals (x_0, x_1) and (x_∞, x_1), we determined the matrices $Y_0(x_1)$ and $Y_\infty(x_1)$. The condition of continuity of the function $\varphi_i(x)$ and $\varphi_i'(x)$ at $x = x_1$ leads to the set of homogeneous equations $\{Y_0(x_1) - Y_\infty(x_1)\}\varphi(x_1) = 0$, which has a nontrivial solution under the condition

$$\mathrm{Det}\|Y_0(x_1) - Y_\infty(x_1)\| = 0, \qquad (26)$$

whence we can determine R_{cr} at a given charge ζ. In view of Eq. (24), it is natural to choose the matching point at $x_1 = 1$; in numerically solving Eq. (25), it is convenient to make the substitution $t = x^{-1/4}$, $0 < t \le 1$. The choice of the initial points of integration at $x_0 = t_0 = 0.07$ and $x_\infty = t_0^{-4} \approx 4 \times 10^4$ has made it possible to ensure a precision not poorer than 0.15% in calculating $R_{cr}(\zeta)$.

The choice of trial functions in the form (22) will be referred to as an (m, n) approximation. With increasing m or n, the class of trial functions becomes wider and the accuracy of the (m, n) approximation becomes higher, which can be seen from Table 2. The calculations were performed for $(m, n) = (1, 0), (2, 0), (2, 1)$, and $(4, 3)$. The results for the $Z = 90$–100 nuclei are quoted in Table 3.[12] In order to assess the accuracy of various methods, we consider the case of $Z = 92$ (uranium nuclei) in greater detail (see Table 2). In addition to the (m, n) approximations, we present here some more numbers: the R_{cr} value as obtained by the Ritz method [14] and in the monopole approximation (see also Fig. 4), as well as the R_{cr} value deduced in [9] by matching the relevant asymptotic expressions. From Table 2, it can be seen that, with increasing order of the

Table 2. Convergence of the (m, n) approximations in the two-center problem for the Dirac equation

(m, n)	R_{cr}, fm		
	$Z = 184$ (U + U)	$Z = 190$ (U + Cf)	$Z = 200$
(1, 0)	34.7	–	68.1
(2, 0)	37.4	–	72.4
(2, 1)	38.37	50.8	74.4
(4, 3)	38.42	50.9	74.8
According to [24, 25]	36.8	48	–
Asymptotic values from [9]	35.5	46.7	68.2
Monopole approximation [25]	34.1	44.8	64.8

Table 3. Parameters of the $1s\sigma$ electron state at the critical point

$Z_1 = Z_2$	$R_{cr}^{(0)}$		R_{cr}	A_∞	β	ρ
	numerical	asymptotic				
90	31.0	28.7	26.5	2.23	0.807	1.478
92	38.4	35.5	34.3	2.51	0.823	1.426
93	42.4	39.1	38.4	2.66	0.832	1.400
94	46.6	42.8	42.6	2.82	0.840	1.376
95	50.9	46.7	47.0	2.99	0.848	1.353
96	55.4	50.8	51.6	3.17	0.857	1.330
97	60.0	55.0	56.3	3.36	0.865	1.307
98	64.8	59.2	61.0	3.56	0.873	1.286
99	69.7	63.7	66.0	3.76	0.881	1.265
100	74.8	68.2	71.1	3.98	0.888	1.244
114	160.0	143.0	–	3.98	0.888	–
126	255.0	–	–	–	–	–

Note: The distances $R_{cr}^{(0)}$ (for pointlike nuclei) and R_{cr} (with allowance for finite nuclear sizes) are given in fm. The former were obtained from a numerical calculation in [23] and from the asymptotic formula (32). The parameters β and ρ are defined in (30a) and (31), respectively.

[11] The expressions for the coefficients $P_{ij}(x)$, etc., for $x < 1$ differ from those for $x > 1$ because the topology of the surfaces $x(\xi, \eta) = c$ changes at $c = 1$: they are simply connected for $c > 1$ and doubly connected for $0 < c < 1$.

[12] Unfortunately, an algebraic error was made in [22] in calculating the coefficients Q_{13} and Q_{23} in the equations of the (2, 1) approximation [these terms die out at small and large distances from nuclei and do not affect the corresponding asymptotic expressions for $\psi(\mathbf{r})$; therefore, they are poorly controllable]. This error resulted in overestimating the R_{cr} values in the (2, 1) approximation by about 20% (see [23, 24] in this connection); however, it exerts no effect on the (1, 0) and the (2, 0) approximation, where the results from [22] remain valid.

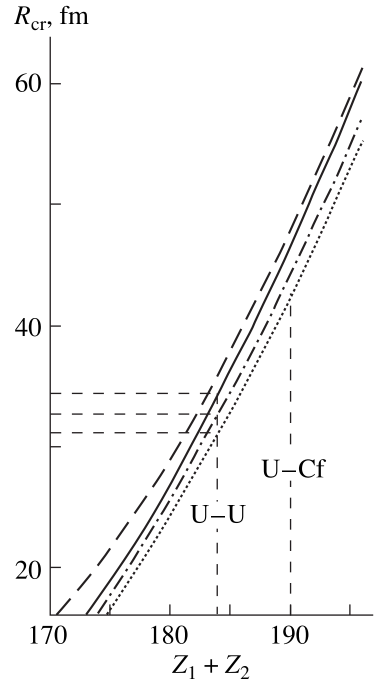

Fig. 4. Critical radius R_{cr} (fm) for the $1s\sigma$ ground-state term according to [25]: (dashed curve) results for naked nuclei at $r_N = 0$, (solid curve) results for naked nuclei with allowance for finite nuclear sizes, (dash-dotted curve) results for the case of 30 electrons in the atomic shell, and (dotted curve) results for the case of 100 electrons in the atomic shell.

(m, n) approximation, the relevant values of R_{cr} increase monotonically {from the variational principle, it follows that the exact value of R_{cr} can only exceed the result obtained in any (m, n) approximation [8, 18]}.

Let us now consider the Ritz method. In these calculations, use was made of a system of the Hilleraas basis functions

$$\psi^m_{nls}(\xi, \eta) = \exp\left(-\frac{\xi-1}{2a}\right)L^m_n\left(\frac{\xi-1}{a}\right)P^m_l(\eta)\chi_s, \quad (27)$$

which leads to a fast convergence in the nonrelativistic problem of two centers. However, these functions are finite near the nuclei ($\xi \longrightarrow 1$, $\eta \longrightarrow \pm 1$), whereas an exact solution to the relativistic problem of two centers has a Coulomb singularity:

$$\psi(\mathbf{r}) \propto (\xi^2 - \eta^2)^{-\sigma}, \quad \sigma = 1 - \sqrt{1-(Z\alpha)^2/4}, \quad Z = Z_1 + Z_2 \quad (28)$$

(in the nonrelativistic limit $Z\alpha \longrightarrow 0$, this singularity disappears). The presence of the singularity impairs convergence of the expansion in the basis $\{\psi^m_{nls}\}$. Within the Kantorovich method, there is no such difficulty, since the functions $\varphi_k(x)$ automatically have the required singularity for $x = \xi^2 - \eta^2 \longrightarrow 0$ [this is ensured by the set of Eqs. (23) itself]. In all probability,

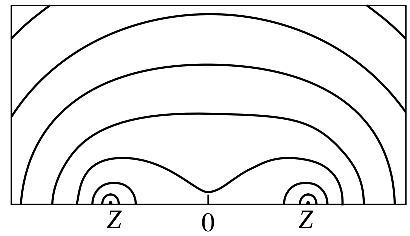

Fig. 5. Density ρ_{cr} for the $1s\sigma$ ground-state term at $Z_1 = Z_2 = 92$. The values of ρ_{cr} for neighboring curves differ by the factor of $10^{1/5}$. The positions of the nuclei are denoted by Z.

this explains the fact that, for $Z = 92$, the R_{cr} value as obtained within the Ritz method with 100 trial functions is close to the result from [22] in the (1, 0) approximation, which involves only one function $\varphi_1(x)$.

It is also possible to compute the electron wave function at the critical point $\zeta = \zeta_{cr}$ and quantities associated with it (see [23] and Appendix C of the present study). Figure 5 shows the density $\rho_{cr}(\mathbf{r}) = \psi^+\psi$ for the $1s\sigma$ state of the U + U quasimolecule at $R = R_{cr}$. Near each nucleus, as well as at large distances from the nuclei, the density $\rho(\mathbf{r})$ is spherically symmetric; that is,

$$\rho_{cr}(\mathbf{r}) \approx \begin{cases} A_0^2 r_i^{2(\sigma-1)}, & r_i \longrightarrow 0 \ (i = 1, 2), \\ A_\infty^2 r^{-3/2}\exp(-\sqrt{32\zeta r}), & r \longrightarrow \infty, \end{cases} \quad (29)$$

where $\sigma = \sqrt{1-\zeta^2/4}$. The asymptotic coefficients A_0 and A_∞ were computed in [23]. Table 3 gives the values of the coefficient A_∞, which determines the probability of peripheral processes (for example, the probability of atom ionization in a strong electric field).

Near the boundary $\varepsilon = -1$, the energy of the level is

$$\varepsilon(R) = -1 + \beta\frac{R - R_{cr}}{R_{cr}} + O((R - R_{cr})^2). \quad (30)$$

The slope parameter β, which determines the threshold behavior of the cross section for spontaneous positron production [4, 21], can be calculated by the formula

$$\beta = \frac{1}{2}\left(\frac{d\ln R_{cr}}{d\zeta}\right)^{-1}\int\psi^+\left(\frac{1}{r_1} + \frac{1}{r_2}\right)\psi d^3r, \quad \psi = \begin{pmatrix}\varphi \\ \chi\end{pmatrix}. \quad (30a)$$

The results are quoted in Table 3. For nuclei from the uranium region, β is a nearly linear function of Z (Fig. 6). The values of the parameter

$$\rho = \int\chi^+\chi d^3r/\int\varphi^+\varphi d^3r, \quad (31)$$

which characterizes the magnitude of relativistic effects for a bound electron, are also given in Table 3.

Finally, the approximate analytic formula

$$R_{cr}(\zeta) = \zeta^{-1}\exp\left\{\frac{1}{g}\left[\arg\Gamma(1+2ig) - \operatorname{arccot}\frac{g-g'/g}{1+g'}\right]\right\} \qquad (32)$$

was obtained in [9] by matching the relevant asymptotic expressions for the problem of two centers.[13)] This method is usually quite accurate for shallow levels—this can be easily demonstrated by considering the problem of two delta-function wells at a fixed distance between them (the simplest example of a two-center problem). Therefore, it is natural to apply it to the problem being considered because, here, the effective energy is $E = 0$.

In (32), we set $g = \sqrt{\zeta^2-1}$, $g' = \sqrt{4-\zeta^2}$, and $\zeta = (Z_1 + Z_2)/137$ and denoted by $\arg\Gamma(z)$ that branch of this multifunction for which $g^{-1}\arg\Gamma(1 + 2ig) = -2C + O(g^2)$ for $g \longrightarrow 0$ ($C = 0.5772\ldots$). This simple formula qualitatively reproduces the ζ dependence of the critical distance. It is consistent with expression (11) for $\delta \longrightarrow 0$ and, as can be seen from Tables 2 and 3, has an uncertainty of about 5 to 10% for $Z_1 + Z_2 \lesssim 200$ (as Z increases beyond this value, its accuracy deteriorates, however). Surprisingly, the asymptotic expression (32) agrees, to a percent precision, with the R_{cr} values as calculated with allowance for finite nuclear sizes (see Table 3); therefore, it can be used to obtain a fast estimate of R_{cr}.

For the case of scalar particles, a similar approximation was constructed in [8], where the authors also formulated the variational principle for calculating R_{cr}. For the case of one spherical nucleus, they found that Z_{cr} satisfies the equation

$$r_N = \frac{1}{2\zeta_{cr}}\exp\left\{\frac{1}{g}\left[\arg\Gamma(1+2ig) - \operatorname{arccot}\left(-\frac{\xi}{g}\right)\right]\right\}, \qquad (32a)$$

where $g = \sqrt{\zeta_{cr}^2 - 1}$ and ξ is the same quantity as in Eq. (6). A comparison of expression (32a) with the results of the calculations according to the exact Eq. (6) reveals that, in the region around $r_N \sim 10$ fm, this formula provide ζ_{cr} to a percent precision.

The last row of Table 2 presents R_{cr} values calculated in the monopole approximation, which corresponds to replacing the potential (18) by its zeroth spherical harmonic:

$$V(\mathbf{r}) \longrightarrow V_0(r) = \frac{1}{4\pi}\int V(r\mathbf{n})d\Omega_{\mathbf{n}}. \qquad (33)$$

For the two-center problem ($r_N = 0$, $Z_1 = Z_2$), we have $V_0(r) = -2\zeta/R$ for $0 < r < R/2$ and $V_0(r) = -\zeta/r$ for $r > R/2$.

[13)] In order to derive this formula, use was made of the fact that an excess over the critical charge is small in actual collisions: $\delta = (Z_1 + Z_2 - Z_{cr})/Z_{cr} \ll 1$ (for example, $\delta = 0.07$ in U + U collisions and $\delta \approx 0.1$ in U + Cf collisions).

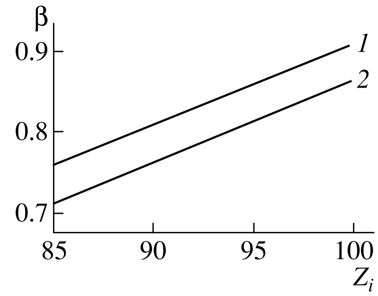

Fig. 6. Slope β of a level in the two-center problem [see Eq. (30)] versus the ion charge Z_i: (straight line *1*) results of the numerical calculation according to formula (30a) and (straight line *2*) results in the WKB approximation [formula (A.7)].

With allowance for finite nuclear sizes and at $Z_1 \neq Z_2$, the expression for $V_0(r)$ is rather cumbersome {see Eq. (29) from [25])}, but numerically solving the Dirac equation presents no serious difficulties because of the spherical symmetry of the potential. It can be seen from Table 2 that, for nuclei from the uranium region, the precision of the monopole approximation is acceptable (about 10%). The critical-distance values obtained in this way in [25] are displayed in Fig. 4 both for naked nuclei and for nuclei with an electron shell featuring 30 and 100 electrons.

So far, we have considered the $1s\sigma$ ground-state term of the relevant quasimolecule. For the next, $2p_{1/2}\sigma$, term, the result in the monopole approximation at $Z_1 = Z_2 = 92$ is $R_{cr} \approx 18$ fm [25], which is close to the sum of the radii of the two nuclei involved. In this case, the deformation of one nucleus by the Coulomb field of the other nucleus becomes sizable, so that the problem ceases to be pure.

4. EFFECTIVE-POTENTIAL METHOD

The effective-potential method [7, 18] is useful for a qualitative analysis of the situation that emerges when a discrete level approaches the boundary of the lower continuum. The method consists in going over from the Dirac equation to the simpler Schrödinger equation featuring an effective energy E and an effective potential U. In general, the relation between the effective potential U and the original potential V directly appearing in the Dirac equation is rather complicated. The relevant expressions are simplified at the boundary of the lower continuum because, there, we are dealing with states at zero (effective) energy ($E = 0$). Equation (3) then takes the form

$$U(r) = -\frac{1}{2}V^2 - V + \frac{\kappa^2+\kappa}{2r^2} + \frac{1}{4}v' - \frac{\kappa v}{2r} + \frac{1}{8}v^2, \qquad (34)$$

where $v(r) = -V'/V$ depends only on the form of the original potential $V(r)$. Let us consider some specific examples.

For power-law attractive potentials

$$V(r) = -gr^{-\nu} \quad \text{for} \quad 0 < r < \infty\ (\nu > 0), \qquad (35)$$

we have $v(r) = \nu/r$; taking into account the Langer correction $1/8r^2$, which improves the accuracy of the semiclassical approximation at small distances [40],[14] we arrive at

$$U(r) = -\frac{g^2}{2r^{2\nu}} + \frac{g}{r^\nu} + \left(\kappa + \frac{1-\nu}{2}\right)^2 \frac{1}{2r^2}. \qquad (35a)$$

By way of example, we indicate that, in the case of a Coulomb field, the effective potential has the form

$$U(r) = \frac{\zeta}{r} - \frac{\zeta^2 - \kappa^2}{2r^2} \quad (g = \zeta, \nu = 1) \qquad (36)$$

(see Fig. 7). Thus, we conclude that, for ε values close to –1, the effective potential involves a broad Coulomb barrier, owing to which the electron state under analysis is not delocalized when $\varepsilon \longrightarrow -1$; that is, the wave function decreases fast at infinity (compare with the results presented in [1]). For example, relation (17) holds at the critical point $Z = Z_{cr}$. This distinguishes the problem being considered from a typically nonrelativistic situation, where $\psi(r) \sim e^{-\lambda r}$ and $\lambda = \sqrt{2m\varepsilon_b} \longrightarrow 0$ for $\varepsilon_b \longrightarrow 0$ (here, ε_b is the binding energy—that is, the spacing between the level and the boundary of the continuous spectrum).

The presence of a Coulomb barrier in the effective potential affects all features of spontaneous positron production. For $Z > Z_{cr}$, the 1s level disappears from the discrete spectrum, going over to the lower continuum.[15] Since $\varepsilon < -1$, the effective energy E is positive, so that there arises the possibility for the level to decay by penetrating through the potential barrier (see Fig. 7). The penetrability of the barrier in the effective potential determines the probability $\gamma(k)$ of spontaneous positron production. At the threshold ($k \ll 1$, where $k = \sqrt{\varepsilon_0^2 - 1}$ is the emitted-positron momentum), we have [3, 4]

$$\gamma \propto \exp\{-2\pi\zeta[\sqrt{1+k^2}/k - \sqrt{1-\zeta^{-2}}]\} \approx \exp\left(-b\sqrt{\frac{Z_{cr}}{Z - Z_{cr}}}\right) \qquad (37)$$

(apart from a preexponential factor), where b is a numerical factor on the order of unity—for example, $b = 1.73$ for model I at $\zeta_{cr} = 1.25$.

For arbitrary $\nu < 2$, the potential in (35a) involves a barrier whose penetrability is exponentially small when $k \longrightarrow 0$. By using the Wentzel–Kramers–Brillouin (WKB) method,[16] one obtains [69, 70]

$$\begin{aligned} \psi_0(r) &\propto [U(r)]^{-1/4} \exp\left\{-\int^{r} \sqrt{2U(r')}\,dr'\right\} \\ &\propto r^{\nu/4} \exp\left(-\frac{\sqrt{8g}}{2-\nu} r^{\frac{2-\nu}{2}}\right), \\ & r \longrightarrow \infty, \end{aligned} \qquad (38)$$

$$\gamma(k) \propto \exp\{-\sqrt{\pi}\Gamma((2-\nu)/2\nu)/\Gamma(\nu^{-1}) k^{\nu}\}. \qquad (39)$$

But if $\nu > 2$, the penetrability here is determined by the centrifugal barrier; at the threshold, we therefore have

$$\gamma(k) \propto k^L, \quad L = j + \frac{1}{2}(1 - \nu\,\mathrm{sgn}\,\kappa).$$

Let us finally consider short-range potentials featuring an exponential tail,

$$V(r) = -gr^{-\nu}\exp(-\mu r), \quad r \longrightarrow \infty. \qquad (40)$$

From (34), we find in this case that

$$U(r) = \frac{1}{8}\mu^2 + \frac{(\nu - 2\kappa)\mu}{4r} + O\left(\frac{1}{r^2}\right), \quad \varepsilon = -1; \qquad (41)$$

therefore, we have $\psi_0(r) \propto \exp(-\mu r/2)$. Thus, we conclude that a state that descends to the boundary of the lower continuum remains localized in this case as well.

The use of an effective potential proved to be very useful for developing a physical interpretation of electron states occurring in a lower continuum for $Z > Z_{cr}$ [7].

Finally, we would like to comment on higher spin ($s > 1/2$) particles. Solutions to the Proca equation ($s = 1$) in the Coulomb field of a pointlike charge were considered in [71, 72], and it was shown there that, for any $\zeta > 0$, there occurs a collapse into the center. For the attractive potentials $V(r) = -gr^{-n}$ ($n > 0$), the effective

[14] It is well known that, in some cases, semiclassical energy spectra become coincident with exact ones upon introducing this correction.

[15] According to [1], the charge density associated with a single electron is delocalized for $Z \longrightarrow Z_{cr}$. However, the preexponential factor that appears in the asymptotic expression for the wave function, $\psi(r) \propto r^{\mu}\exp(-\lambda r)$, and which is associated with the Coulomb barrier in the effective potential (36) was disregarded in [1]. Since $\mu = \zeta\varepsilon/\lambda \longrightarrow -\infty$ and $\lambda = \sqrt{1-\varepsilon^2} \longrightarrow 0$ for $\varepsilon \longrightarrow -1$, the factor r^{μ} compensates for an ever slower decrease of the exponential $\exp(-\lambda r)$ for $r \longrightarrow \infty$, when the level approaches the boundary of the lower continuum (in contrast to the case of $\varepsilon \longrightarrow -1$, where the Coulomb interaction of the electron with the nucleus increases $\langle r \rangle$ in relation to what occurs in the case of a short-range potential). Thus, a bound state at the boundary of the lower continuum remains localized both for electrons [3] and for scalar mesons [4]. Therefore, there are no reasons to expect that the polarization charge of the vacuum increases greatly for $Z \longrightarrow Z_{cr}$ (in the case of fermions, for which the Pauli exclusion principle is operative [7]); this is fully confirmed by the numerical calculations of vacuum polarization that were performed in the 1980s, as well as by those calculations for the vacuum-polarization-induced shifts of levels in heavy atoms up to $Z = 137$ and even up to $Z = 170 \sim Z_{cr}$.

[16] The condition of applicability of the semiclassical approximation [41, 47] is satisfied here: $\frac{d}{dr}(1/p(r)) \propto \nu g^{-1/2} r^{-(2-\nu)/2} \ll 1$ for $r \longrightarrow \infty$.

potential (35) for states characterized by specific values of the total angular momentum j has the form

$$U(r) = -gn\sqrt{j(j+1)}/r^{n+2} + \ldots, \quad r \longrightarrow 0; \tag{42}$$

therefore, collapse into the center occurs here at an arbitrarily small power-law singularity of $V(r)$ at the origin [3]. For the Proca equation, the potential that represents the boundary between regular and singular potentials has the form

$$V(r) = -g\ln\frac{1}{r} + \ldots, \quad r \longrightarrow 0, \tag{43}$$

in which case

$$U(r) = -g\sqrt{j(j+1)}/r^2 + \ldots. \tag{44}$$

For $g < g_{\rm cr} = (j+1/2)^2/\sqrt{j(j+1)}$, this potential is regular, requiring no cutoff; as soon as the coupling constant g exceeds the critical value $g_{\rm cr}$, it becomes singular (similarly to the Coulomb potential for the Dirac and the Klein–Gordon equation).

5. WENTZEL–KRAMERS–BRILLOUIN METHOD FOR $Z > 137$

It is of interest to apply the semiclassical approximation to the case of a strong Coulomb field. The first attempt along these lines was made by Krainov [73], but he used the WKB method not only in the Coulomb field region ($r > r_N$) but also in the interior of the nucleus, where its accuracy is rather poor. A consistent application of the WKB method to the relativistic Coulomb problem was developed in [74], where the semiclassical wave function was matched with a solution to the Dirac equation in the internal region ($0 < r < r_N$). In practice, it is more convenient to find not $\zeta_{\rm cr}$ at a given nuclear radius but the function

$$r_N = \frac{\zeta_{\rm cr}^2 - \kappa^2}{\zeta_{\rm cr}(1+\cosh 2y)},$$

$$y - \tanh y = \frac{1}{2\sqrt{\zeta_{\rm cr}^2 - \kappa^2}} \tag{45}$$

$$\times\left\{\left(n_r + \frac{2l+3}{4}\right)\pi - \operatorname{arccot}\left(\frac{\xi}{\sqrt{\zeta_{\rm cr}^2-\kappa^2}}\right)\right\},$$

where ξ is the logarithmic derivative of the internal wave function at the boundary of the nucleus (see Appendix A). This formula is convenient for applications, its accuracy is about 1% in the region of radii around $r_N \sim 10$ fm, and it correctly reproduces the dependence of $Z_{\rm cr}$ on the model of cutoff of the Coulomb potential within the nucleus (see Fig. 1). Moreover, its accuracy only improves with increasing r_N or $\zeta_{\rm cr}$ [see Fig. 1 and Eq. (A.4)]. For the next, $2s_{1/2}$, level, the precise and the semiclassical curve are indistinguishable on the scale of the figure.

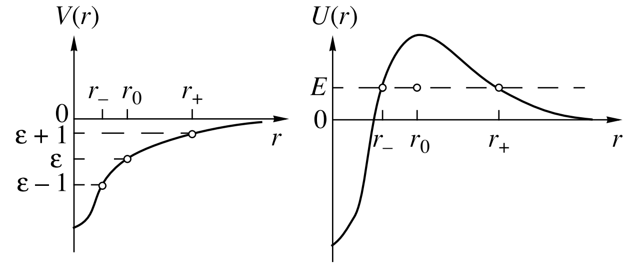

Fig. 7. Original potential $V(r)$ and effective potential $U(r)$ for the relativistic Coulomb problem at $Z \approx Z_{\rm cr}$ [here, $r_\pm$ are the turning points, while $r_0 = (\zeta^2 - \kappa^2)/\zeta$ is the point where the effective potential peaks].

The electron state at the boundary of the lower continuum remains localized [see Eqs. (17) and (29) above]. Therefore, the discrete level for $Z \longrightarrow Z_{\rm cr}$ does not tend to be tangent to the boundary $\varepsilon = -1$, entering the lower continuum with a finite slope β:

$$\varepsilon(\zeta) = -1 + \beta(\zeta_{\rm cr} - \zeta) + \ldots. \tag{46}$$

The value of β is of some interest for the theory [4, 21]. As can be seen from Figs. 3 and 6, the WKB method determines the slope parameter β to a satisfactory precision.

The semiclassical approximation can also be applied to the relativistic two-center problem. Referring the interested reader to [75–77] for details, where the WKB method was consistently developed for $\varepsilon \approx -1$ states of the Dirac equation, we only present here an equation that determines the energies of the electron terms of the quasimolecular system (Z_1, Z_2, e^-) near the boundary $\varepsilon = -1$. Specifically, we have

$$\frac{R_{\rm cr}}{R} = \left[1 - \left(1 + \frac{1-2\kappa}{4\zeta^2}\right)(1+\varepsilon)\right]\phi(x), \tag{47}$$

where

$$x = (1-\rho^2)\left[\varepsilon^2 - 1 + \left(\kappa - \frac{5}{4}\right)\frac{(1+\varepsilon)^2}{\zeta^2}\right]$$

$$\times\left[1 - \left(1 + \frac{1-2\kappa}{4\zeta^2}\right)(1+\varepsilon)\right]^{-2},$$

$$\phi(x) = \exp\left\{\frac{1}{2\sqrt{x}}[(1+\sqrt{x})\ln(1+\sqrt{x})\right.$$

$$\left. - (1-\sqrt{x})\ln(1-\sqrt{x})] - 1\right\}, \quad x > 0,$$

$\phi(x) = (1-x)^{1/2}\exp\{(\arctan\sqrt{-x}/\sqrt{-x}) - 1\}, \quad x < 0,$

$\zeta = (Z_1 + Z_2)/137$, and $\rho = |\kappa|/\zeta$ $(0 < \rho < 1)$. At $\varepsilon \approx -1$, we have $x = (1-\rho^2)(\varepsilon^2 - 1) + \ldots$. According to (47), the energy of the term, ε, depends on the ratio $R/R_{\rm cr}$ [this is a corollary of the condition $r_N \ll r \ll r_K$ (where r_K is the K-shell radius), which is satisfied, provided that the

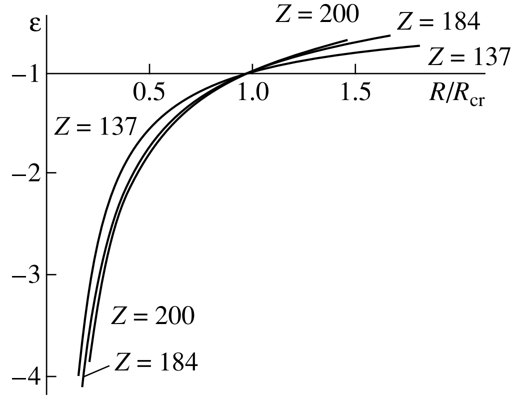

Fig. 8. Energy of the ground-state term in the two-center problem. The values of the total charge $Z = Z_1 + Z_2$ of the nuclei involved are indicated on the curves.

total charge of the two nuclei involved exceeds only slightly the critical charge value, $Z_1 + Z_2 - Z_{cr} \ll Z_{cr}$]. The value R_{cr} itself was calculated separately—for example, by means of the variational method (see Section 3). The results are represented by the curves in Fig. 8.

The possible existence of $Z \gg Z_{cr}$ nuclei (of course, stability of such nuclei can be ensured only by some new mechanism—for example, by the formation of a negative-pion condensate [28]), referred to as supercharged ones, was considered in the literature [29, 78]. We denote by n_κ and N the number of discrete levels characterized by a given value of the quantum number κ that have descended to the lower continuum and the total number of such levels, respectively, and by N_e the number of electrons in the vacuum shell of a supercritical atom (such a shell is formed near a supercritical atom upon positron emission). Obviously, the relations $N = \sum_\kappa n_\kappa$ and $N_e = \sum_\kappa (2j + 1)n_\kappa$ then hold; in the semiclassical approximation, we obtain

$$N = \frac{1}{2}\int_0^\infty (V^2 + 2V)_+ r\,dr,$$
$$N_e = \frac{4}{3\pi}\int_0^\infty \{(V^2 + 2V)_+\}^{3/2} r^2\,dr, \tag{48}$$

where $f_+(r) = f(r)$ if $f(r) \geq 0$ and $f_+(r) = 0$ if $f(r) < 0$. In the case of the potential given by (5), it follows that, for $\zeta \gg 1$, we have

$$N = \frac{1}{2}\zeta^2\left(\ln\frac{\zeta}{r_N} + c_4\right),$$
$$N_e = \frac{4}{3\pi}\zeta^3\left(\ln\frac{\zeta}{r_N} + c_5\right), \tag{49}$$

where c_4 and c_5 are numerical constants on the order of unity that depend on the cutoff model. Figure 9 borrowed from [79] demonstrates that the semiclassical approximation is quite accurate even at relatively small values of $\zeta \gtrsim 2$.

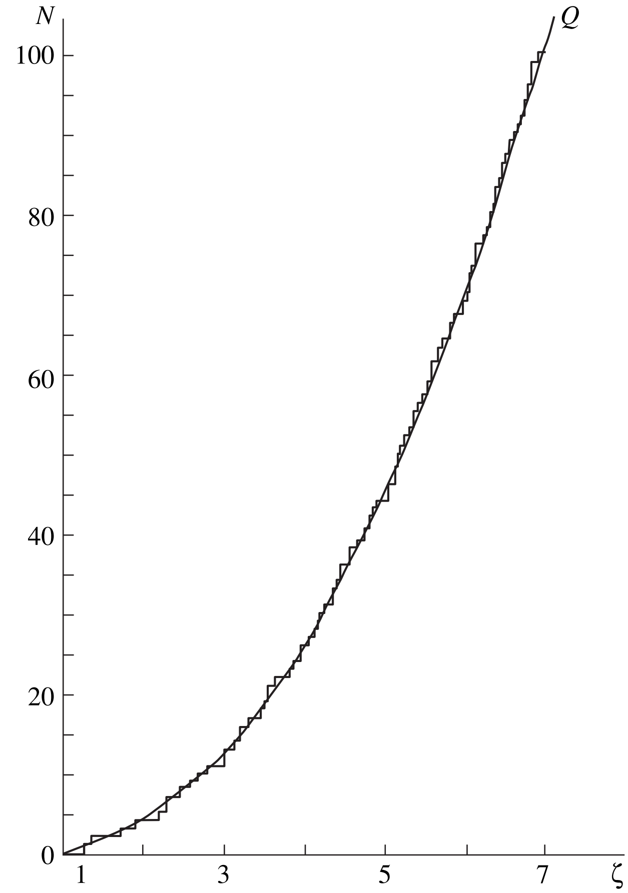

Fig. 9. Number N of levels that have descended to the lower continuum [for the potential (5)]. The stepwise broken line represents a numerical solution to the Dirac equation, while the curve Q was computed according to the semiclassical formula (49).

Equations (48) suggest that the local density of the electron cloud in the vacuum shell of a supercritical atom is $\rho(r) = (V^2 + 2V)^{3/2}/3\pi^2$, and this natural assumption can indeed be rigorously substantiated [54]. This makes it possible to write the relativistic Thomas–Fermi equation [26, 54]

$$\Delta V = -4\pi e^2\left[\frac{1}{3\pi^2}(V^2 + 2V)^{3/2} - n_p(r)\right] \tag{50}$$

(where n_p is the density of protons in a supercritical nucleus), whose solution determines the properties of the electron shell in an atom for $Z \gg 137$.

We will not dwell any more on these questions, referring the interested reader to the aforementioned studies and to the monographs [38, 39, 78]. The only objective here was to demonstrate the efficiency of the WKB method for ultrastrong Coulomb fields.

Table 4. Accuracy of the WKB method for the Salpeter equation (case of massless quarks)

	$n_r = 0$	1	2	3	5	References
$l = 0$	0.9724	0.9958	0.9983	0.9991	0.99953	[83]
	0.9725	0.9959	0.9982	0.99905	–	[84]
$l = 1$	0.9391	0.9743	0.9858	0.9908	0.9952	[83]
	0.9382	0.9744	0.9859	0.9910	–	[84]
$l = 2$	0.9232	0.9590	0.9742	0.9820	0.9897	[83]
$l = 3$	0.9152	0.9478	0.9642	0.9742	–	[84]

Note: Quoted in the table are the meson-mass ratios $M_{n_r l}^{(\text{calc})}/M_{n_r l}$, where $M_{n_r l}$ stands for the results of numerical calculations from [83, 84], while $M_{n_r l}^{(\text{calc})}$ corresponds to the calculation relying on the modified quantization rule from [74] and taking into account relativistic kinematics according to [85].

It should be noted here that the WKB method can be applied to two-particle relativistic wave equations, including the Salpeter equation [80–82] for the quark–antiquark system. In the case of the confining potential $V(r) = \sigma r$ (where σ is the tension of the string between the quark and the antiquark involved) in this Salpeter equation

$$\{\sqrt{\mathbf{p}^2 + m_1^2} + \sqrt{\mathbf{p}^2 + m_2^2} + V(r)\}\psi_n = M_n\psi_n,$$

where $\mathbf{p} = -i\nabla$, m_1 and m_2 are the masses of the quarks (whose spins are disregarded here), and M_n are the meson masses, the semiclassical mass spectrum of mesons agrees, to a percent accuracy, with the spectrum obtained by numerically solving [83, 84] the Salpeter equation (especially for $l \sim 1$ states, including the ground state, for which $n_r = l = 0$). For further details, the reader is referred to [85, 86] (see also Table 4).

6. Z_{cr} FOR OTHER PARTICLE SPECIES

In the case of a Coulomb field, the Klein–Gordon equation has a solution decreasing at infinity,

$$\chi_l(r) = \text{const} \times W_{\mu,\, i\nu/2}(x), \quad -1 \le \varepsilon < 1, \tag{51}$$

where $x = 2\lambda r$,

$$\lambda = \sqrt{1-\varepsilon^2}, \quad \mu = \zeta\varepsilon/\lambda, \\ i\nu/2 = \sqrt{(l+1/2)^2 - \zeta^2}, \tag{51a}$$

and $W_{\mu,\, i\nu/2}$ is the Whittaker function. The energy of the ground-state level in the field of a pointlike charge is

$$\varepsilon_0(\zeta) = \left(\frac{1}{2} + \sqrt{\frac{1}{4} - \zeta^2}\right)^{1/2} = \frac{1}{\sqrt{2}}\left(1 + \sqrt{\frac{1}{2} - \zeta} + \dots\right), \\ \zeta \longrightarrow \frac{1}{2} \tag{52}$$

[compare with Eq. (1)]. States that are pure in the orbital angular momentum l now undergo collapse into the center for $\zeta > l + 1/2$. In the limit $\varepsilon \longrightarrow -1$, which corresponds to $\lambda \longrightarrow 0$, $\mu \longrightarrow -\infty$, and $\mu x \longrightarrow -2\zeta r$, the Whittaker function is simplified significantly to become

$$\chi_l(r) = \text{const} \times r^{1/2} K_{i\nu}(\sqrt{8\zeta r}), \\ \nu = 2\sqrt{\zeta^2 - (l+1/2)^2}. \tag{53}$$

It can easily be shown that the equation for ζ_{cr} can be written in a unified form for the spin values of $s = 0$ and 1/2; that is,

$$zK'_{i\nu}(z)/K_{i\nu}(z) = 2(s+\xi) - 1, \tag{54}$$

where $z = \sqrt{8\zeta_{\text{cr}} r_N}$, as in Eq. (6). For the ground state, we have $\nu = 2\sqrt{\zeta_{\text{cr}}^2 - (s+1/2)^2}$ in both cases.

Under the condition $r_N \ll 1/m$, we have $\xi = \zeta \cot\zeta$ for the cutoff model I (see Appendix A), as before. Considering, however, that $mr_N > 1$ for pions, we conclude that the Klein–Gordon equation must be solved exactly in the internal region $r < r_N$. In the simplest case ($l = 0$, cutoff model I), we obtain

$$\xi = \beta\cot\beta, \quad \beta = \sqrt{\zeta(\zeta - 2r_N)}. \tag{55}$$

Equations (54) and (55) were solved with the aid of a computer [3]. Although $Z_{\text{cr}} = 1/2\alpha = 68.5$ for a pointlike charge in this case, the value of Z_{cr} exceeds 137 even at $r_N \sim 0.1\hbar/mc$ (see Fig. 4 in [3]). A numerical calculation for pions ($\hbar/m_\pi c$ = 1.41 fm) yields $Z_{\text{cr}}^{(\pi)} \approx 3300$ [87], which is far beyond any known nucleus.

The situation is similar for muons ($\hbar/m_\mu c$ = 1.87 fm). Solving Eq. (6) led to $\zeta_{\text{cr}} = 16.7$ or $Z_{\text{cr}}^{(\mu)} \approx 2300$ for model II and $Z_{\text{cr}}^{(\mu)} \approx 3700$ for model I [69]. Thus, we can see that, for $r_N \ll 1/m$, the numerical value of Z_{cr} depends greatly on the choice of model. It should be emphasized that it was Migdal who suggested the existence of supercharged nuclei with $Z \sim 137^{3/2}$ [29]; however, the theory does not provide definitive results

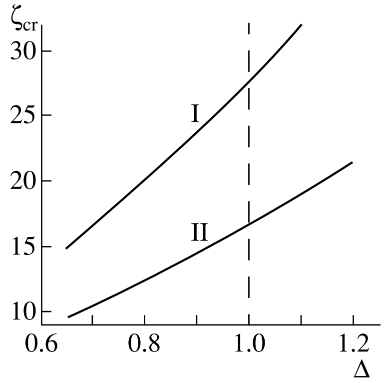

Fig. 10. Critical charge of a nucleus for the muon (the cutoff models I and II were used). For ordinary heavy nuclei, the parameter Δ is equal to unity.

for their density and for the relation between A and Z. Let us assume that $r_N = r_0 A^{1/3}$, where $r_0 = 1.2\delta$ fm and $A/Z = 2.6\xi$, δ and ξ being free parameters (for conventional nuclei, we have $\delta = \xi = 1$). The critical charge $Z_{cr}^{(\mu)}$ depends strongly on the parameter $\Delta = \delta\xi^{1/3}$ (see Fig. 10). It should also be noted that the above values of the critical charge should be treated as a first approximation, since the calculation took no account of the screening of the potential (5) by the electron shell that the naked nucleus attracts from a vacuum upon the spontaneous emission of positrons and their escape to infinity. The inclusion of the screening effect is expected to increase Z_{cr} still further.

Thus, the situation where muon or pion levels in a superheavy nucleus reach the boundary $\varepsilon = -mc^2$ can hardly be realized.

7. MISCELLANEA

Here, we consider some additional questions related to those discussed in Sections 2–6.

1. From Eq. (4), it can be seen that, for $\varepsilon \approx -1$, $\zeta > j + 1/2$ electron states, an effective attraction proportional to $1/r^2$ arises at small distances (for a pointlike charge, it leads to a collapse into the center [46–49]). This attraction, which is a purely relativistic effect, stems from introducing the Coulomb interaction of the electron with the nucleus in a minimal way—that is, through the time component of the 4-potential A_μ. This can be seen from the example of the Klein–Gordon equation alone, which is obtained for a spinless particle from the relation $\mathbf{p}^2 = \varepsilon^2 - m^2$ by means of the substitution $p_\mu \longrightarrow p_\mu - eA_\mu$. The resulting equation

$$\Delta\varphi + [(\varepsilon - V)^2 - m^2]\varphi = 0 \qquad (56)$$

is identical to the Schrödinger equation in form if we set

$$E = (\varepsilon^2 - m^2)/2m, \quad U = \frac{\varepsilon}{m}V - \frac{1}{2m}V^2. \qquad (57)$$

The term $-\frac{1}{2m}V^2$ is dominant at small distances, where $|V(r)| \longrightarrow \infty$ and leads to attraction, irrespective of the sign of $V(r)$. For the spin value of $s = 1/2$, the form of the effective potential becomes more complicated, but it undergoes no significant qualitative changes: the expression for $U(r)$ develops additional terms associated with the particle spin and spin–orbit interaction [see Eqs. (3) and (34) and also Appendix C].

2. If light charged scalar bosons (of mass about m_e) existed in nature, then effects associated with the approach of a discrete level to the boundary $\varepsilon = -mc^2$ would be observable because $Z_{cr} = 68.5$ at $r_N = 0$ for such bosons. However, we have $\hbar/m_\pi c = 1.41$ fm and $m_\pi r_N \gg 1$ for the pion, and Z_{cr} considerably exceeds 137 in this region, as was shown in the preceding section.

A modest (in relation to the case of a pointlike charge) increase in Z_{cr} from $Z_{cr}^{(0)} = 137$ for electrons is associated with the fact that $m_e r_N \sim 0.03 \ll 1$.

3. With increasing potential-well depth, the energy levels ε for bosons and fermions behave differently, which was first discovered by Schiff *et al.* [88], who considered the example of s states in the square well $V(r) = -g\theta(r_0 - r)$ for the Klein–Gordon equation. Namely, the dependence of ε on the coupling constant g in the case of the Klein–Gordon equation is nonmonotonic—there is a backbending, which occurs near $\varepsilon = -1$ if the well is sufficiently wide. At some coupling-constant value $g = g_{cr}$, two levels going from the continuum boundaries $\varepsilon = 1$ and -1 merge, whereupon there arise states characterized by a square-integrable wave function; however, the energies of these states are complex-valued, which is at odds with unitarity. This means that, at $g > g_{cr}$, the single-particle Klein–Gordon Hamiltonian is no longer a self-conjugate operator and has no physical meaning.

A physical interpretation of this phenomenon was given by Migdal [28]: at $g \sim g_{cr}$, there occur the virtual production of charged particle–antiparticle pairs and a strong vacuum polarization, which screens the bare charge g, thereby preventing it from reaching the critical charge g_{cr}. It follows that, in the boson case, the theory must inevitably be multiparticle at $g \sim g_{cr}$. (For electrons, the situation is totally different. Because of the Pauli exclusion principle, there are only two vacancies in the K shell at $Z > Z_{cr} \sim 170$ upon positron emission; therefore, vacuum polarization leads only to a small effect of order α and is unable to prevent the descent of the next levels of the electron spectrum to the lower continuum [7].)

By developing these considerations further, Migdal *et al.* [78] created the theory of pion condensation in nuclear matter and predicted some interesting effects. Unfortunately, no experimental evidence for the existence of a pion condensate in conventional heavy nuclei has been obtained so far.

4. It should be noted that the problem of establishing the character of the motion of levels near the boundary $\varepsilon = -1$ presents considerable difficulties, because its investigation involves analyzing complicated equations. After [88], the problem was addressed in [89–95]; however, some of the results presented in [91, 92] are erroneous. The relativistic generalization of the effective-range expansion for states whose energy is close to the boundary of the lower continuum is a very convenient means for studying this problem [95]. An analysis along these lines reveals [69, 95] that, for the Dirac equation, there are no positron levels that would arise from the lower continuum and which would have a positive derivative $d\varepsilon/d\zeta$. At the same time, there are such levels for the Klein–Gordon equation [88], in which case, for a short-range potential $V(r) = -gv(r)$, two bound states merge at some value $g = g_{cr}$ and $\varepsilon > -1$; for $g > g_{cr}$, the S matrix for this case develops complex poles on the physical sheet. A remarkable property of the Dirac equation is that it does not involve such a difficulty; therefore, the single-particle Dirac equation retains, to some extent, its meaning in the supercritical region $g > g_{cr}$ as well [7].

If the potential $V(r)$ possesses a Coulomb tail for $r \longrightarrow \infty$, the bound state remains localized even at $\varepsilon = -1$ and $\zeta = \zeta_{cr}$ owing to the presence of a barrier in $U(r)$ [see Eq. (17) above]. Therefore, all levels of the discrete spectrum enter the lower continuum at a finite slope $d\varepsilon/d\zeta = -\beta < 0$ (both for the spin of $s = 1/2$ and for the spin of $s = 0$ [4]). Nonetheless, the distinction between the boson and the fermion case still remains at the fundamental level: the S-matrix pole corresponding to a bound state at $Z < Z_{cr}$ goes into the complex plane (for $Z > Z_{cr}$) on the physical sheet at $s = 0$ and on the unphysical sheet at $s = 1/2$.

5. Let us consider the effect of a magnetic field on Z_{cr}. In a magnetic field so strong that the Larmor radius of an electron, $l = \sqrt{\hbar c/eB} = \sqrt{B_0/B}$ (in $\hbar/mc$ units), is less than the mean ground-state radius $\langle r \rangle$, the electron shell is squeezed toward the nucleus in the direction orthogonal to the field $\mathbf{B}$, taking a cigarlike shape [96–98]; therefore, the electron effectively undergoes a stronger attraction to the nucleus than in the absence of a field, whereby the critical charge decreases. The condition $l \ll \langle r \rangle$ actually corresponds to $B \gg B_0 = m^2c^3/e\hbar = 4.41 \times 10^{13}$ G (where B_0 is the critical, Schwinger [99], field[17]) peculiar to QED).

The problem being discussed was comprehensively studied in [101]. For a "weak" magnetic field, the reduction of Z_{cr} can be found by perturbation theory. The result is

$$\zeta_{cr}(B) = \zeta_{cr}(0) - \frac{5\pi^2\mu}{6[\ln(1/r_N)]^3}\frac{B}{B_0} + O((B/B_0)^2), \quad (58)$$

where μ is the magnetic moment (15). It follows that, even at $B \sim 0.1B_0 \sim 5 \times 10^{12}$ G, $\Delta Z_{cr} < 1$.

For stronger fields, the dependence $Z_{cr}(B)$ is obtained from the equations derived in [101], which were solved numerically. Presented immediately below are some results referring to the ground state: $Z_{cr} \approx 165$ at $B = B_0$, $Z_{cr} = 96$ at $B = 100B_0$, $Z_{cr} = 92$ (uranium nucleus) at $B = 133B_0 \approx 5.5 \times 10^{15}$ G, and $Z_{cr} = 41$ at $B = 2.4 \times 10^4 B_0 \approx 10^{18}$ G. The next level of the electron spectrum reaches the boundary $\varepsilon = -1$ at $B \sim 1.5 \times 10^{16}$ G if $Z_{cr} = 92$, and so on.

Thus, we conclude that, in the presence of a strong magnetic field, the boundary of the lower continuum can be reached at charge values as small as $Z < 170$—for example, in the case of a naked uranium nucleus or even in the case of lighter nuclei. The above estimates show, however, that this requires magnetic fields of strength not less than the critical one. It should be recalled that maximum magnetic fields achieved so far under laboratory conditions are six orders of magnitude less than that [102, 103].

6. Some authors considered modifications to QED and their effect on spontaneous positron production.[18]) In particular, Rafelski *et al.* [107] considered a nonlinear Lagrangian of the Born–Infeld type [108]. For the case of electrostatics, it leads to the energy density

$$w = \frac{E_0^2}{2n}\left[\left(1 + \frac{D^2}{E_0^2}\right)^n - 1\right], \quad (59)$$

where n and E_0 are parameters of the theory—for example, $n = 1$ (or $E_0 \longrightarrow \infty$), $n = 1/2$, and the limiting case of $n = 0$ correspond, respectively, to Maxwell electrodynamics, to Born–Infeld theory, and to Infeld–Hoffmann theory.

We denote by E_B the E_0 value obtained from the condition [108] that the electron mass is entirely of an electromagnetic origin. We then have $E_B = 1.2 \times 10^{18}$ V/cm at $n = 1/2$, in which case $Z_{cr} = 214$ for the $1s$ level [107]. This would naturally dash the hopes for observing spontaneous positron production in experiments with known heavy nuclei. However, the above value of E_0 contradicts experimental data on atomic levels. In order to avoid a conflict with the precisely measured energy differences in the spectra of the ^{82}Pb and ^{100}Fm nuclei, it is necessary to assume [110] that $E_0 > 140E_B \sim 2 \times 10^{20}$ V/cm. As a result, the critical charge can increase by not more than two units.

Here, we will not consider other modifications to QED (see, for example, [111, 112]) that were also discussed in the literature in connection with the effect of spontaneous positron production.

[17]) Of course, so strong a field can occur only under extremal conditions (for example, within pulsars [100]).

[18]) At present, the predictions of QED are in remarkable agreement with experimental data: in the record case of the electron anomalous magnetic moment, the accuracy is 10^{-12} [104–106]. In this connection, the modifications to QED that are discussed below seem less interesting.

7. The method of linear combinations of atomic orbitals (LCAO), which is known from quantum chemistry, was used in [113] to solve the relativistic two-center problem. For the ground-state term considered in the case of identical charges of the nuclei involved, one can set

$$\psi = a\psi_1 + b\psi_2, \quad a = b = 1/\sqrt{2(1+S)}, \qquad (60)$$

where ψ_1 and ψ_2 are the wave functions of an electron moving in the field of, respectively, the first and the second center, while $S = \langle\psi_1|\psi_2\rangle$ is the overlap integral. The relativistic wave functions of the hydrogen-like atom [45] with an effective charge $Q\alpha < 1$ (which depends on R and Z) were taken for ψ_1 and ψ_2. As a result, an analytic, albeit rather cumbersome, formula was obtained for the ground-state term. This formula makes it possible to calculate $\varepsilon_0(R, Z)$ over a wide region of R and Z. A comparison with the numerical results from [27] shows that the error of this formula is 10% at $Z/2 = 35$ (Br + Br system) and as large as 25% at $Z/2 = 92$. Thus, we can see that, in the region $90 \leq Z/2 \leq 100$, the accuracy of this approximation is insufficient, so that it is necessary to use a more complicated trial function featuring a greater number of variational parameters than in (60).

8. OPTIMISTIC CONCLUSION

Qu'est-ce qu'optimisme? disait Cacambo.
Hélas! dit Candide, c'est la rage de soutenir
que tout est bien quand on est mal.
Voltaire "Candide ou l'Optimisme"[19)]

Let us briefly touch upon the currently prevalent experimental situation.

Experiments seeking spontaneous and induced positron production in heavy-ion collisions (at energies close to the height of the Coulomb barrier) were performed at the UNILAC heavy-ion accelerator of GSI (Darmstadt, Germany). There, beams of Pb and U ions of energies 3 to 6 MeV per projectile nucleon were obtained. Even the first experiments [114, 115], which were conducted in the subcritical region ($Z_1 + Z_2 < Z_{cr}$), recorded induced positron production due to the quickly varying (in time) Coulomb field of colliding nuclei (the term "quasiatomic" or "induced" positrons is often used in the literature for this case). The energy spectra of these positrons comply well with the results of theoretical calculations for the process. Of particular interest are the results [116–118] presented by two experimental groups, EPOS and ORANGE, which were named after the magnetic spectrometers that they used. In addition to the theoretically predicted continuous spectrum of positrons, these groups reported the observation of a few relatively narrow positron peaks (of width not greater than 40 keV). Later on, this effect, which was much to the surprise of experimentalists and which was dubbed the Darmstadt effect, was repeatedly tested and refined, and a few tens of events were recorded under the areas of the most pronounced peaks (at $E_{e^+} \approx 255$ and 340 keV). Subsequently, narrow peaks were also observed in the spectrum of electrons recorded in coincidence with positrons and in the total-energy ($E_{e^+} + E_{e^-}$) spectra (see [119–121] and references in the review article by Pokotilovsky [122]), which is puzzling phenomenon indeed.

Naturally, these unusual phenomena inspired keen interest of theorists. In the period from 1985 to 1992, there appeared a few tens of theoretical studies that were devoted to the subject and which put forth various hypotheses, sometimes exotic ones, to explain the Darmstadt effect: the decay of a new particle (axion [123, 124]), composite extended particles, magnetic quasibound states of the e^+e^- system [125], a new phase in the QED vacuum [112], the formation (in heavy-ion collision) of a quasimolecule whose nuclei are at a distance $R < R_{cr}$ for a time period $T \gg R_{cr}/v \sim \hbar/mc^2 \sim 10^{-21}$ s [126, 127], and the capture and cooling of positrons in an expanding open resonator between two Coulomb centers [128]. Without further extending this list, we only note that none of these mechanisms could provide a full and compelling description of all phenomena observed at GSI.

More recently, a critical analysis of these (extremely difficult) experiments and new experiments that collected much vaster statistics revealed that narrow lines in the electron and positron spectra were an experimental error (this was recognized by the authors from GSI themselves [129, 130]), so that no new physics is needed, as has already occurred many times in the history of science, for explaining these phenomena.

It is difficult to say when the Darmstadt experiment will be continued, if at all, and when a detailed comparison of the theory of spontaneous positron production with experimental data will be performed, which would imply a check upon QED and upon the Dirac equation not in the traditional region of high energies and small distances but in the new region of ultrastrong external fields. These experiments are complicated[20)] and expensive, while one should not expect sensational discoveries here. At the same time, such experiments do not require new giant accelerators whose construction

19)"What is optimism?" said Cacambo. "Alas!" Candide said, "it is the mania of maintaining that everything is well when we are wretched." [Quoted from *Candide and Other Romances by Voltaire* (Dodd, Mead and Company, New York, 1928; translated from the French by Richard Aldington.]

20)The main difficulty here consists in isolating the process of interest among other processes inevitably accompanying it, like induced positron production and the formation of positrons in nuclear processes. Moreover, the spontaneous-positron-production cross section itself is small near the threshold ($E \longrightarrow E_{thr} = 2(Ze)^2/R_{cr}$) [4, 7, 21] because of the Coulomb barrier in (36), which also ensures a localization of the electron state with energy $\varepsilon \leq -1$ in the lower continuum. At energies $E \gtrsim 2E_{thr}$, however, this cross section no longer has an exponential smallness.

could ruin the budget of a country: the energy that is necessary to cause the approach of two uranium nuclei within the critical distance of $R_{cr} \approx 35$ fm is 5 to 6 MeV per nucleon, an energy value that has long since been achieved at heavy-ion accelerators available worldwide. Moreover, considerable advances have recently been made in producing beams of heavy ions deprived partly or even completely of their electron shell (it should be recalled [7, 38, 39] that, for spontaneous positron production, it is necessary that an unfilled K-level descend to the lower continuum[21)]). All this gives sufficient grounds to regard the future of experimental investigations in these realms of physics with a refrained optimism (at the same time, the above opinion of Voltaire also deserves attention).

The situation can change drastically if $Z \gtrsim 137^{3/2}$ nuclei are discovered some day, which must be surrounded, as the theory indicates, by a dense vacuum shell consisting of electrons that have descended to the lower continuum. The possible existence of such supercharged nuclei (with $A > 10^3$ and $N = Z$) was repeatedly emphasized by Migdal [29, 78, 131–133]. Their stability would be guaranteed owing to the screening of the proton charge by the negative-pion condensate and by electrons distributed within the nucleus:

"For $Z > Z_c \approx (137)^{3/2}$ stable nuclei should exist. At a sufficient value of $Z - Z_c$ such nuclei should be stable with respect to fission" [29].

"For highly charged nuclei, fission instability is most important. Fission stability is possible only if the Coulomb energy is considerably suppressed. This means that the π^- charge should be of the order of Z. As we have shown, $Z_\pi \approx Z$ at $Ze^3 \sim 1$. Thus, the considerable suppression of the Coulomb energy at $Ze^3 \sim 1$ can lead to the stability of supercharged nuclei" [133].

An analysis has revealed that there exist two possible regions of stability of anomalous nuclei—the region of superdense nuclei ($Z \approx N$, $Z \lesssim 10^2$) and the region of superheavy nuclei ($Z \approx N$, $Z \gtrsim 10^3$); here, the electric charge of baryons is fully compensated by the pion condensate and by the electrons …. In the limiting case of $Z \gg 1/e^3 \approx 1600$, the interior of a superheavy nucleus appears to be an electrically neutral plasma formed by baryons, pion-condensate mesons, electrons, and negative muons. For such nuclei, there are no upper bounds on A, so that there can in principle exist stars in the form of a nucleus [78].

These are basic conclusions from those studies on the possible existence of superheavy nuclei in nature. Of course, it should be borne in mind that the modern theory of the nucleus is not celestial mechanics: even the law of interaction between two nucleons in a vacuum has not been established conclusively, nor can an *ab initio* solution to the Schrödinger equation for a heavy nucleus be obtained. Therefore, a theoretical extrapolation from conventional nuclei to the far region around $Z \sim 137^{3/2}$ can hardly be reliable.[22)] However, we would like to complete the present discussion with the following words: "Cela est bien dit, répondit Candide; mai il faut cultiver notre jardin" [136].[23)]

[21)]It is worthy of note that spontaneous positron production from a vacuum is possible not only in a collision of two $Z_u > Z_{cr}$ nuclei with unfilled K shells but also in the case where this is so for only one (Z_1) of the nuclei (the second can involve K electrons—this can be for example, a neutral atom of the target nucleus). In the latter case, it is necessary that $Z_1 \geq Z_2$, as follows from a comparison of the molecular terms of the (Z_1, Z_2, e) system at small and at large distances between the nuclei [20, 21].

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APPENDIX A

Semiclassical Approximation in the Relativistic Coulomb Problem

(a) Let us consider the case of a heavy spherical nucleus. Since we have $r_N \ll \hbar/mc = 1$ in Eq. (5) (at $\zeta = 1.25$, the nuclear radius is $r_N \approx 0.023$), the main contribution to the quantization integral comes from the region $r_N < r < r_0$, where

$$p^2(r) = \frac{g^2}{r^2}\left(1 - \frac{r}{r_0}\right), \quad g = \sqrt{\zeta^2 - \kappa^2}, \qquad r_0 = g^2/2\zeta, \tag{A.1}$$

r_0 being the turning point. The semiclassical wave function corresponding to the upper component of the Dirac

[22)]In this connection, the following comment is in order. Estimates from [28, 131] revealed that there are nuclei close to the pion-condensate instability; in particular, pion condensation may occur in ordinary heavy nuclei. However, a detailed analysis of experimental data (absence of the doubling of the 0^+ and 0^- levels in the ^{208}Pb spectrum, which is known comprehensively; probabilities of single-nucleon slow-pion capture by nuclei; etc.) showed that there is no condensate in nuclei [78, 134]. At present, the variational calculations from [135] indicate that pion condensation is possible in neutron stars [at a density of $\rho \sim (1.5\text{–}2.0)\rho_0$, where $\rho_0 \approx 0.15$ nuclon/fm^3 is the normal nuclear density].

[23)]"It is well said," replied Candide, "but we must cultivate our gardens." [Quoted from *Candide and Other Romances by Voltaire* (Dodd, Mead and company, New York, 1928; translated from the French by Richard Aldington.]

bispinor has here the form

$$G(r) = [rp(r)]^{-1/2}\sin\left(\int_{r_N}^{r} p(r')dr' + \gamma\right).$$

The phase γ is determined by matching this wave function with the internal wave function at the boundary of the nucleus. The result is

$$g\cot\gamma = \xi + O(r_N/r_0), \quad \xi = \left.\frac{d\ln G(r)}{d\ln r}\right|_{r = r_N} \tag{A.2}$$

(actually, we have $r_N/r_0 \lesssim 0.1 \ll 1$). For ζ_{cr}, the modified quantization condition [74] yields

$$\int_{r_N}^{r_0} \sqrt{\frac{\zeta_{cr}^2 - \kappa^2}{r^2} - \frac{2\zeta_{cr}}{r}} = \left(n_r + \frac{2l+3}{4}\right)\pi - \gamma, \tag{A.3}$$
$$n_r = 0, 1, 2, \ldots.$$

Upon evaluating the integral, Eq. (A.3) reduces to the form (45). It should be noted that the greater ζ, the higher the degree to which the condition

$$\frac{d}{dr}(1/p(r)) = \frac{1 - r/2r_0}{g(1 - r/r_0)^{3/2}} \ll 1, \tag{A.4}$$

which ensures the applicability of the semiclassical approximation, is satisfied (this is so everywhere with the exception of the vicinity of the turning point). This explains the behavior of the curves in Fig. 1.

(b) Let us consider the relativistic problem of two centers. For nuclei from the uranium region, the radius of the K shell is five to ten times as great as R_{cr}; in calculating the energy $\varepsilon(R)$ of the electron term, it is therefore not necessary to know the wave function in the region $r \lesssim R/2$, where the special features of the two-center problem are of importance, but where the ε dependence of $p(r)$ is immaterial. Equation (47) for $\varepsilon(R)$ follows from a comparison of two quantization integrals at close energies. We have

$$\int_{R/2}^{r_t} F(r, \varepsilon)\frac{dr}{r} = \int_{R_{cr}/2}^{r_0} F(r, \varepsilon = -1)\frac{dr}{r}, \tag{A.5}$$

where $p(r) = r^{-1}F(r, \varepsilon)$ is a semiclassical momentum,

$$F = [a - 2br + cr^2 + O((1+\varepsilon)^3)]^{1/2},$$
$$a = g^2 = \zeta^2 - \kappa^2,$$
$$b = \zeta\left[1 - \left(1 + \frac{1 - 2\kappa}{4\zeta^2}\right)(1 + \varepsilon)\right], \tag{A.6}$$
$$c = \varepsilon^2 - 1 + \left(\kappa - \frac{5}{4}\right)\zeta^{-2}(\varepsilon + 1),$$

and $r_t = r_0\left[1 - \frac{1}{2}(1 - \kappa^2/\zeta^2)(1 + \varepsilon) + \ldots\right]$ is the position of the turning point at ε values sufficiently close to –1.

In Eq. (47), we have $x = 0$ at $\varepsilon = -1$; the function $\phi(x)$ is given by different formulas for $x > 0$ and $x < 0$, but $x = 0$ is not a singular point for this function: $\phi(x) = 1 - \frac{1}{6}x + O(x^2)$ for $x \longrightarrow 0$. A compact expression for the slope parameter β can be obtained from Eq. (47) [77]. The result is

$$\beta = \frac{3}{2}\left(1 + \frac{4\kappa^2 - 6\kappa + 3}{8\zeta^2}\right)^{-1}. \tag{A.7}$$

In particular $\beta = 12\zeta^2/(8\zeta^2 + 13)$ for the ground-state term (see straight line *2* in Fig. 6).

(c) The logarithmic derivative ξ appearing in Eqs. (6), (54), (A.2), and (A.3) can be found from the Riccati equation [18]

$$u' - \left(\frac{f'}{f} + \frac{1}{x}\right)u + \frac{u^2}{x} = \frac{\kappa(\kappa+1)}{x} + \kappa\frac{f'}{f} - \zeta^2 x f^2, \tag{A.8}$$
$$0 < x < 1.$$

We also have $\xi = u(1)$ and $u(0) = |\kappa|$ if $\kappa < 0$ [here, $x = r/r_N$, and $f(x)$ is the cutoff function from Eq. (5)]. For the $\kappa = j + 1/2 > 0$ states, we obtain

$$\xi(\zeta, \kappa) = \zeta^2/[\kappa - \xi(\zeta, -\kappa)] - \kappa. \tag{A.9}$$

For example, we find for the *ns* levels ($\kappa = -1$) within model I that

$$\xi(\zeta, -1) = \zeta\cot\zeta$$
$$= \sum_{k=0}^{\infty} a_k\zeta^{2k} = 1 - \frac{1}{3}\zeta^2 - \frac{1}{45}\zeta^4 - \frac{2}{945}\zeta^6 - \ldots, \tag{A.10}$$

where $a_k \approx -2/\pi^{2k}$ for $k \longrightarrow \infty$; for $\kappa = -(l + 1) < 0$, we have

$$\xi(\zeta, \kappa) = (2l+1)\frac{f_l(\zeta)}{f_{l+1}(\zeta)} - l$$
$$= l + 1 - \frac{\zeta^2}{2l+3} - \frac{\zeta^4}{(2l+3)^2(2l+5)} + \ldots, \tag{A.11}$$

while for $\kappa = l > 0$, we use Eq. (A.9). In particular, we find for the $np_{1/2}$ states that

$$\xi(\zeta, 1) = \zeta^2 - 1 + \frac{\zeta^3}{\tan\zeta - \zeta}$$
$$= 2 - \frac{1}{5}\zeta^2 - \frac{1}{175}\zeta^4 - \ldots, \tag{A.12}$$

where l is the orbital angular momentum for the upper component and $f_l(x) = \Gamma(l + 1/2)(x/2)^{1/2 - l}J_{l-1/2}(x)$, $f_l(0) = 1$. For more realistic cutoff models, it is straightforward to calculate the values of ξ numerically.

Presented below are some useful expansions. Representing the volume charge density in a nucleus as

$$\frac{Z}{4\pi r_N^3}\rho(r/r_N), \quad \int_0^1 \rho(x)x^2 dx = 1, \tag{A.13}$$

and setting $\rho(x) = \rho_0 + \rho_1 x + \rho_2 x^2 + \ldots$, we arrive at

$$\begin{aligned} f(x) &= f_0 - \sum_{n=2}^{\infty} \frac{\rho_{n-2}}{n(n+1)} x^n, \\ f_0 &= \int_0^1 \rho(x) x dx = \sum_{n=0}^{\infty} \frac{\rho_n}{n+2}. \end{aligned} \tag{A.14}$$

By way of example, we indicate that, for the $\kappa = -1$ states, the result for ξ is

$$\begin{aligned} \xi &= 1 - c_1\zeta^2 - c_2\zeta^4 + \ldots, \\ c_1 &= \sum_{n=0}^{\infty} \frac{(n+6)}{3(n+3)(n+5)}\rho_n. \end{aligned} \tag{A.15}$$

In particular, we find for model II that $\rho(x) = 3\theta(1-x)$, $\rho_0 = 3$, and $\rho_n = 0$ for $n \geq 1$ and that $a_1 = 2/5$, $a_2 = 17/40$, $a_3 = 0.665$, ….

In the case of scalar particles, it is only necessary to replace $\kappa(\kappa+1)$ by $l(l+1)$ in Eq. (A.8) and to discard terms involving $f'(x)$. For the cutoff model I, the value of $\xi(\zeta, l)$ is then coincident with that in (A.11).

APPENDIX B

The energy eigenvalues for the Dirac equation with the pointlike-charge potential $V(r) = -\zeta/r$ are given by [45]

$$\varepsilon_{nj\kappa} = \sqrt{1 - \zeta^2/N^2}, \quad N = \sqrt{q^2 + q\nu + \kappa^2}, \tag{B.1}$$

where $q \equiv n_r = 0, 1, 2, \ldots$ is the radial quantum number; n is the principal quantum number; $\nu = 2\sqrt{\kappa^2 - \zeta^2}$; and $j = 1/2, 3/2, \ldots, n - 1/2$ is the angular momentum. The mean radius of the $|nj\kappa\rangle$ state is [6] is

$$\langle r \rangle_{nj\kappa} = \frac{1}{2\zeta}[(3N^2 - \kappa^2)\varepsilon_{nj\kappa} - \kappa], \quad \zeta < |\kappa|. \tag{B.2}$$

In particular, expression (13) follows from here for the ground-state ($n = N = 1$) level; for the energy-degenerate (at $\zeta < 1$) $2s_{1/2}$ and $2p_{1/2}$ levels, we have[24)]

$$\begin{aligned} \varepsilon_2(\zeta) &= [(1 + \sqrt{1-\zeta^2})/2]^{1/2}, \\ \langle r \rangle &= \frac{1}{2\zeta}(12\varepsilon_2^3 - \varepsilon_2 - \kappa). \end{aligned} \tag{B.3}$$

[24)]It should be emphasized, however, that, at $\zeta \approx 1$, these formulas, as well as those in (1) and (13), are valid to a logarithmic precision [see (10)].

For the $\kappa = \pm 1$ states, there is a square-root singularity at $Z = 137$ [see, for example, Eq. (1a)],

$$\langle r \rangle = \frac{1}{2}\left[\frac{q(3q^2+2)}{\sqrt{q^2+1}} \pm 1\right] + O(\sqrt{1-\zeta^2}), \tag{B.4}$$

where $q = n - 1$ and where the upper (lower) sign refers to the $ns_{1/2}$ ($np_{1/2}$) states.

It is natural to determine the magnetic moment of an electron in a bound state from the relation $\mu = -(\partial\varepsilon/\partial B)_{B\to 0}$, where $\delta\varepsilon = \left\langle -\frac{1}{2}[\mathbf{r}\alpha]\cdot\mathbf{B}\right\rangle$. This yields (in Bohr magneton units) [6]

$$\mu = [1 + (2j+1)\varepsilon]/(2j+2), \quad \kappa < 0, \tag{B.5}$$

and a similar formula for $\kappa > 0$ states.

In the particular case of $\kappa = -n$ (that is, for the $1s_{1/2}$, $2p_{3/2}$, $3d_{5/2}$, etc., states, including the ground state), the relevant formulas are simplified to become

$$\begin{aligned} \varepsilon_n &= \sqrt{1 - \frac{\zeta^2}{n^2}}, \quad \langle r \rangle = \frac{n}{2\zeta}(1 + 2\sqrt{n^2 - \zeta^2}), \\ \mu &= \frac{1 + 2\sqrt{n^2 - \zeta^2}}{2n+1} \end{aligned} \tag{B.6}$$

(the formula for μ was obtained by Breit [137]).

For the ground state of $s = 0$ or $s = 1/2$ particles, the probability-distribution density and its moments are given by

$$\rho(r) = \psi^+\psi = A^2 \exp(-2\lambda r) r^{2\eta - 2}, \tag{B.7}$$

$$\langle r^\sigma \rangle = 4\pi\int_0^\infty \rho(r) r^{\sigma+2} dr = \frac{\Gamma(2\eta + \sigma + 1)}{(2\lambda)^\sigma \Gamma(2\eta + 1)}, \tag{B.8}$$

where

$$\lambda = \sqrt{1 - \varepsilon^2}, \quad \eta = \varepsilon\zeta/\lambda, \quad A = \sqrt{\frac{2^{2\eta-1}\lambda^{2\eta+1}}{\pi\Gamma(2\eta+1)}},$$

and $\varepsilon = \varepsilon_0(\zeta)$ is the energy of this state. In particular, we have

$$\begin{aligned} \langle r \rangle &= \frac{2\eta + 1}{2\lambda}, \quad \Delta r = (\langle r^2 \rangle - \langle r \rangle^2)^{1/2} = \frac{\sqrt{2\eta+1}}{2\lambda}, \\ \left\langle \frac{1}{r} \right\rangle &= \frac{\lambda}{\eta}, \quad \langle V \rangle = -\zeta\langle 1/r \rangle = -(1 - \varepsilon_0^2)/\varepsilon_0, \\ \langle T \rangle / \langle V \rangle &= -(1 + \varepsilon_0)^{-1} \end{aligned} \tag{B.9}$$

($\varepsilon_0 = m + \langle T \rangle + \langle V \rangle$). Thus, the virial theorem $\langle V \rangle = -2\langle T \rangle$ is valid only for $\zeta \ll 1$—that is only in the nonrelativistic case.

Table 5

ζ_{cr}	$\kappa = -1$			$\kappa = 1$		
	ρ	$\langle r\rangle$	μ_{cr}	ρ	$\langle r\rangle$	μ_{cr}
1.00	2.33	0.130	0.133	0.333	0.075	0
1.25	1.61	0.312	0.354	0.333	0.195	0
1.50	1.22	0.447	0.533	0.333	0.300	0

For $s = 1/2$ (electron), we have $\varepsilon_0 = \eta = \sqrt{1-\zeta^2}$ and $\lambda = \zeta$, while, for scalar particles, the results are

$$\varepsilon_0 = \left(\frac{1}{2} + \sqrt{\frac{1}{4} - \zeta^2}\right)^{1/2},$$

$$\lambda = \left(\frac{1}{2} - \sqrt{\frac{1}{4} - \zeta^2}\right)^{1/2}, \quad \eta = \varepsilon_0^2.$$

In the nonrelativistic limit, we arrive at

$$\varepsilon_0(\zeta) = 1 - \frac{\zeta^2}{2} - \frac{a}{8}\zeta^4 + \dots,$$
$$\lambda = \zeta + \frac{a-1}{8}\zeta^3 + \dots, \quad \eta = 1 - \frac{a+3}{8}\zeta^2 + \dots, \tag{B.10}$$

$$A = \sqrt{\frac{\zeta^3}{\pi}}\left[1 - \frac{a+3}{8}\zeta^2 \ln\zeta + O(\zeta^2)\right],$$
$$\langle r\rangle = \frac{3}{2Z}a_B\left(1 - \frac{5a+3}{24}\zeta^2 + \dots\right), \tag{B.11}$$

where $a = 1$ at $s = 1/2$ and $a = 5$ at $s = 0$, while $a_B = \hbar^2/me^2$ is the Bohr radius.

If $\zeta \geq j + 1/2$, the pointlike-nucleus approximation is no longer applicable to states characterized by the angular momentum j; as a result, the wave functions become much more complicated [3, 5]. At $\varepsilon = -1$, we can use, however, the simpler expressions (16). For $ns_{1/2}$ ($\kappa = -1$) states, this leads to expressions (14) and (15), while, at $\kappa = 1$, we arrive at

$$\langle r\rangle = \frac{3}{40\zeta_{cr}}(4\zeta_{cr}^2 - 3), \quad \mu_{cr} = 0. \tag{B.12}$$

It is interesting to note that, for $\zeta_{cr} \gg 1$, the mean radius behaves identically, $\langle r\rangle = 0.3\zeta_{cr}[1 + O(\zeta_{cr}^{-2})]$, in the two cases ($\kappa = \mp 1$).

We denote by w_1 and w_2 the relative weights of the upper and the lower component of the Dirac bispinor (in other words, the probability that a bound electron has the orbital angular moment l or $l' = 2j - l$),

$$w_1 = \int_0^\infty G^2(r)dr = (1+\rho)^{-1},$$
$$w_2 = \int_0^\infty F^2(r)dr = \frac{\rho}{1+\rho}. \tag{B.13}$$

The parameter $\rho = w_2/w_1$ characterizes the degree to which the electron state being considered is relativistic. To illustrate this, we note that, in the nonrelativistic state ($\rho = \zeta^2/4n^2 \ll 1$), we have $\rho = (q + \sqrt{q^2+1})^{-2}$ at $\zeta = 1$ and

$$\rho = \frac{1}{3}\left[1 + \frac{2\kappa^2 - 3\kappa + 1}{\zeta_{cr}^2}\right] \tag{B.14}$$

for states at the boundary of the lower continuum.

It should be emphasized that these formulas are valid only under the condition $r_N \ll \langle r\rangle$. The numerical values of the parameters for $\varepsilon = -1$ states are quoted in Table 5.

The mean radius $\langle r\rangle$ increases quite fast with increasing ζ_{cr}. This increase is not due to the effect of the internal region $r < r_N$, whose contribution is small. The probability for the electron to reside within the nucleus can be roughly estimated as $w_N \approx (r_N/\langle r\rangle)^3 \sim 10^{-3}$–$10^{-2}$ at $r_N = 10$ fm. In this sense, the situation resembles that in the deuteron, with the difference—a significant one, however—that the electron, which is relativistic here ($\rho \sim 1$), is confined near the nucleus owing to the Coulomb barrier in the effective potential (36). The probability w_N can be calculated more precisely by using the formula

$$w_N = \frac{4\pi A_0^2}{2\eta+1}(m_e r_N)^{2\eta+1}, \tag{B.15}$$

where A_0 is the asymptotic coefficient in the wave function at the origin. This yields $w_N = 0.02$, 0.019, and 0.037 for the $1s$, $2s$, and $2p_{1/2}$ states, respectively; for two nuclei at the distance $R = R_{cr}$, we have $A_0 = 3.56$ and w_N 3.6(–3) at $Z/2 = 92$ and $A_0 = 1.86$ and $w_N = 1.7(-3)$ at $Z/2 = 100$ (the values of A_0 were borrowed from [23]).

The decrease in the critical distance because of cutting off the Coulomb potential within the nucleus can be computed by the formula

$$R_{cr} = R_{cr}^{(0)}(1 - \beta^{-1}\Delta\varepsilon), \tag{B.16}$$

where $R_{cr}^{(0)}$ is associated with pointlike nuclei (problem of two centers), β is the slope of the level as given by Eq. (30a), and $\Delta\varepsilon$ is the shift of the level upon taking into account finite nuclear sizes.

By perturbation theory, we find

$$\Delta\varepsilon = 2\pi A_0^2 \zeta \gamma^{-1} r_N^{2\gamma} F(\gamma),$$
$$F(\gamma) = 2\gamma \int_0^1 [x^{-1} - f(x)] x^{2\gamma-1} dx, \quad \text{(B.17)}$$

where $\zeta = 2Z\alpha = 2\sqrt{1-\gamma^2}$. The results for the cutoff models I and II are $F(\gamma) = (2\gamma + 1)^{-1}$ and $F(\gamma) = 3/(2\gamma + 1)(2\gamma + 3)$, respectively. A more precise formula for $\Delta\varepsilon$ can be obtained by matching the wave functions at the boundary of the nucleus. In this way, the R_{cr} values quoted in Table 3 were calculated in [23].

APPENDIX C

The Dirac equation for an electron with a static potential $V(\mathbf{r})$ has the form

$$(\boldsymbol{\sigma} \cdot \mathbf{p})\varphi = W\chi, \quad (\boldsymbol{\sigma} \cdot \mathbf{p})\chi = (W - 2)\varphi, \quad \text{(C.1)}$$

where $W = 1 + \varepsilon - V$, while φ and χ are, respectively, the upper and the lower bispinor component (here, the potential is not assumed to be spherically symmetric). The substitution $\psi = W^{-1/2}\varphi$ reduces Eqs. (C.1) to the form

$$\Delta\psi + (\varepsilon^2 - 1 - 2U)\psi = 0, \quad \text{(C.2)}$$

$$U = \varepsilon V - \frac{1}{2}V^2 + \frac{1}{4W}\Delta V + \frac{3}{8W^2}(\nabla V)^2 + \frac{1}{2W}[\nabla V \times \mathbf{p}] \cdot \boldsymbol{\sigma}. \quad \text{(C.3)}$$

Here, ψ and the effective potential U are both two-component quantities. For $1 > \varepsilon \geq -1$, $W(\mathbf{r})$ is positive for any attractive potential; therefore, a transition from the set of Dirac equations (C.1) to Eq. (C.2) does not involve singularities.[25)] Formally, Eq. (C.2) has the form of the ordinary Schrödinger equation featuring spin–orbit coupling. The difference, however, is that the potential U itself depends (in a rather complicated way) on the energy ε. At the boundary of the lower continuum, $W = -V$, expression (C.3) takes the somewhat simpler form (19). The explicit expressions for the functions $U_{ij}(\mathbf{r})$ can be found in [22].

In calculating the mean radius, the slope of the level at the boundary of the lower continuum, and other similar quantities, it is necessary to normalize the Dirac function. It will now be shown how this can be done without calculating the lower component explicitly. From Eqs. (C.1), we have

$$\chi = W^{-1}(\boldsymbol{\sigma} \cdot \mathbf{p})\varphi = SW^{-1/2}\psi,$$
$$\langle\chi|\chi\rangle = \langle\psi|W^{-1/2}S^+SW^{-1/2}|\psi\rangle, \quad \text{(C.4)}$$

where

$$S = W^{-1}(\boldsymbol{\sigma} \cdot \mathbf{p})W = \boldsymbol{\sigma} \cdot \mathbf{P}, \quad \mathbf{P} = \mathbf{p} - i\mathbf{A},$$
$$\mathbf{A} = \nabla \ln W = -W^{-1}\nabla V,$$
$$S^+S = (\mathbf{P}^+ \cdot \mathbf{P}) + i[\mathbf{P}^+ \times \mathbf{P}] \cdot \boldsymbol{\sigma}$$
$$= \mathbf{p}^2 + \mathbf{A}^2 - \nabla\mathbf{A} - 2[\mathbf{A} \cdot \mathbf{p}] \times \boldsymbol{\sigma}, \quad \text{(C.5)}$$

and $\mathbf{p} = -i\nabla$. Performing integration by parts and using Eq. (C.2), we arrive at the identity

$$\langle f\psi|\mathbf{p}^2|f\psi\rangle = \int \psi^+\{(\nabla f)^2 + (\varepsilon^2 - 1)f^2 - (f^2U + Uf^2)\}\psi d^3r, \quad \text{(C.6)}$$

where $f(\mathbf{r})$ is an arbitrary real-valued function (in our case, $f = W^{-1/2}$). Taking into account the relations

$$\nabla\mathbf{A} = -(\mathbf{A}^2 + W^{-1}\nabla V), \quad [\mathbf{p}, W^\alpha] = -i\alpha W^\alpha \mathbf{A},$$
$$W^{-1/2}[\mathbf{A} \times \mathbf{p}]W^{-1/2} = W^{-1}[\mathbf{A} \times \mathbf{p}],$$

and expression (C.3) for the effective potential, we obtain

$$N \equiv \langle\varphi|\varphi\rangle + \langle\chi|\chi\rangle = \int \psi^+\hat{T}\psi d^3r, \quad \text{(C.7)}$$

$$\hat{T} = 2(\varepsilon - V) + \frac{1}{2W^2}\Delta V + \frac{3}{2W^3}(\nabla V)^2 + \frac{1}{W^2}[\nabla V \times \mathbf{p}] \cdot \boldsymbol{\sigma}. \quad \text{(C.8)}$$

Considered immediately below are some cases where the above formulas can be simplified.

(a) For the central field $V = V(r)$, we have

$$[\nabla V \times \mathbf{p}] \cdot \boldsymbol{\sigma} = r^{-1}V'(r)(\mathbf{l} \cdot \boldsymbol{\sigma}) = -(\kappa + 1)r^{-1}V'(r)$$

and $\Delta V = V'' + 2r^{-1}V'$. Equation (C.3) then reduces to Eq. (3), while Eq. (C.8) yields

$$N = \int_0^\infty (G^2 + F^2)dr$$
$$\equiv \int_0^\infty \left\{2\left(1 - \frac{1}{W}\right) + \frac{V''}{2W^3} + \frac{3}{2W^4}V'^2 - \frac{\kappa V'}{rW^3}\right\}G^2(r)dr, \quad \text{(C.9)}$$

where $G = rg(r)$ and $F = rf(r)$ are radial wave functions. In [18], this formula was obtained directly for spherically symmetric potentials and was used in the calculations.

[25)] In the case of a repulsive potential, $V(\mathbf{r}) > 0$, the function W can vanish and become negative. Instead of (C.2), it is therefore necessary to use the equation that is obtained from the set of Eqs. (C.1) upon the substitution $\chi = (1 - \varepsilon + V)^{-1/2}\psi$.

(b) At the boundary of the lower continuum ($\varepsilon = -1$), we have $W = -V$ and

$$\hat{T} = -2(1+V) + \frac{1}{2V^2}\Delta V - \frac{3}{2V^3}(\nabla V)^2 + \frac{1}{V^2}[\nabla V \times \mathbf{p}] \cdot \boldsymbol{\sigma}. \tag{C.10}$$

It should be noted that, in the problem of two pointlike Coulomb centers, we can omit, in the above formulas, terms that are proportional to the Laplacian ΔV. In order to demonstrate this, we note that $W \propto r^{-1}$ for $r \longrightarrow 0$; hence, $W^{-\alpha}\Delta V \propto r^{\alpha}\delta(\mathbf{r}) \equiv 0$ for any $\alpha > 0$. The same is true for any system of pointlike charges.

(c) At $\varepsilon = -1$ and $V(r) = -\zeta/r$, we have

$$N = \int_0^\infty (G^2 + F^2)dr = 2\int_0^\infty \left(1 - \frac{2\kappa - 1}{4\zeta^2} - \frac{r}{\zeta}\right)G^2 dr. \tag{C.11}$$

Similar identities can be obtained for the moments of the electron-density distribution. They are presented here in the simplest (and the most important) case of $\kappa = -1$. Denoting

$$\langle r^\sigma \rangle = \int_0^\infty (G^2 + F^2) r^\sigma dr \Big/ \int_0^\infty (G^2 + F^2) dr,$$

$$\overline{r^\sigma} = \int_0^\infty G^2 r^\sigma \Big/ \int_0^\infty G^2 dr,$$

we obtain

$$\langle r^\sigma \rangle = \left\{\left(\zeta + \frac{\sigma^2 + 4\sigma + 3}{4\zeta}\right)\overline{r^\sigma} - \overline{r^{\sigma+1}}\right\} \Big/ \left(\zeta + \frac{3}{4\zeta} - \bar{r}\right). \tag{C.12}$$

Thus, the problem reduces to averaging over the upper component $G(r)$ exclusively. For the case of the Coulomb field, we find with the aid of (16) that

$$\overline{r^\sigma} = \frac{\sqrt{\pi}\,\Gamma(\sigma+1)}{2(8\zeta)^\sigma \Gamma(\sigma + 3/2)} \left|\frac{\Gamma(\sigma + 1 + i\nu)}{\Gamma(1 + i\nu)}\right|^2, \quad \sigma > -1. \tag{C.13}$$

For natural values of σ, the last expression reduces to polynomials:

$$\overline{r^\sigma} = \zeta^{-1} P_\sigma(\zeta),$$
$$P_1 = \frac{1}{3}\zeta^2 - \frac{1}{4}, \quad P_2 = \frac{2}{15}\zeta^3 - \frac{1}{10}\zeta, \tag{C.14}$$
$$P_3 = \frac{2}{35}\zeta^4 + \frac{1}{35}\zeta^2 - \frac{3}{56}, \ldots.$$

With the aid of (C.14), we can easily deduce Eqs. (14), (15), and (B.12).

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