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ELECTRONIC STRUCTURE OF SUPERHEAVY ATOMS

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We describe the status of the problem of the electron structure of superheavy atoms with nuclear charge $Z > Z_c$; here $Z_c \approx 170$ is the critical value of the nuclear charge, at which the energy of the ground state of the $1S_{1/2}$ electron reaches the limit of the lower continuum of the solutions of the Dirac equation ($\epsilon = -m_e c^2$). We discuss the dependence of Z_c on the nuclear radius R and on the character of the distribution of the electric charge inside the nucleus, and also the form of the wave functions at Z close to Z_c. Owing to the Coulomb barrier, the state of the electron remains localized at $Z > Z_c$, in spite of the fact that its energy approaches the continuum. An analysis of the polarization of the vacuum in a strong Coulomb field shows that a bare nucleus with supercritical charge $Z > Z_c$ produces spontaneously two positrons and, in addition a charge density with a total of two units of negative charge in the vacuum. The distribution of this density is localized in a region of dimension $r \sim \hbar/m_e c$ at the nucleus. The possibility of experimentally observing the effect of quasistatic production of positrons in the collision of two bare uranium nuclei (i.e., without electrons) is discussed. A brief review is presented of work on the motion of levels with increasing depth of the potential well in other relativistic equations (Kelin-Gordon, Proca, etc.).

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1. FORMULATION OF PROBLEM AND DISCUSSION OF RESULTS

THE question of the electron structure of the atom at $Z\alpha > 1$, and especially when the nucleus has a supercritical charge $Z > 170$, is of great fundamental interest. The quantum theory of electrons, positrons, and electromagnetic field cannot be regarded as complete until this question is made completely clear.

It is not very likely that atoms with such large Z can be synthesized and studied, at least in the nearest future. The boldest assumptions concerning the existence of islands of nuclear stability do not go beyond the magic values Z = 114 and 126 (see the reviews [1-3]). In principle, however, the effect of spontaneous quasistatic positron production at $Z > 170$, predicted by the theory, can be observed in the collision of two bare uranium nuclei (i.e., having no electrons). In any case, the difficulties in the performance of the corresponding experiments do not eliminate the need for obtaining a distinct answer within the framework of the theory of electrons and positrons.

The history of the problem is divided into three stages. In the first, Dirac has shown[4] (see also [5-7]) that in a Coulomb field of a point charge Ze the solution becomes singular at Z = 137. For example, the energy of the lower level $1S_{1/2}$ of the discrete spectrum is

$$\varepsilon_1 = \sqrt{1-\zeta^2}, \tag{1.1}$$

where $\zeta = Ze^2/\hbar c = Z/137$.* At $\zeta = 1$, the energy ϵ_1 reaches zero and the $\epsilon = \epsilon(\zeta)$ curve terminates there (Fig. 1). The expression (1.1) has a square-root singularity at the point $\zeta = 1$; a formal continuation of (1.1) to the region $\zeta > 1$ leads to imaginary values of ϵ_1. It

*Here and throughout we use a system of units with $\hbar = c = m_e = 1$, where m_e is the electron mass. The electron energy ϵ includes the rest energy, so that $\epsilon = 1$ corresponds to a free electron at rest and $\epsilon = 0$ corresponds to a binding energy $m_e c^2 = 1$. The boundary of the lower continuum $\epsilon = -1$ corresponds to a binding energy $2m_e c^2$.

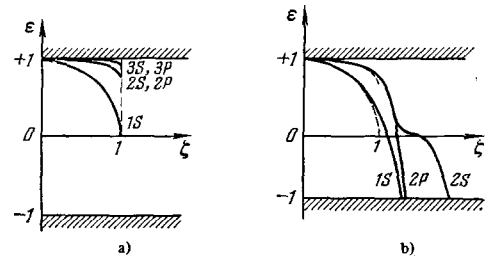

FIG. 1. The energies of the lower levels with angular momentum j = 1/2 ($\zeta = Z/137$): a) for a point-charge potential $V(r) = -Ze^2/r$; b) with allowance for the finite dimensions of the nucleus.

is therefore frequently stated that the Dirac equation has no solution at $Z > 137$ (this, however, is incorrect). In fact, the solution of the Dirac equation in the potential $V(r) = -\zeta/r$ is possible also when $\zeta > 1$, but the problem is incorrectly stated without the choice of the boundary condition on the wave function at zero. The physical meaning of this condition is simply that the problem must be solved with a potential that is cut off at $r < R$.

Taking the finite dimensions of the nucleus into account, Pomeranchuk and Smorodinskiĭ[8] have shown that for an extended nucleus the solution exists from $\zeta = 0$, $\epsilon = 1$ to $\zeta = \zeta_c$, $\epsilon = -1$, and that the singularity of formula (1.1) at $\zeta = 1$ disappears. The value of $Z_c = 137\zeta_c$, at which the energy of the ground state reaches the limit of the lower continuum $\epsilon = -1$, will be called the critical charge of the nucleus. Z_c was calculated in [8] by an approximate method that has low accuracy in the region of real values of the nuclear radius $R \sim 10^{-12}$ cm. Consequently, the values of Z_c given there are too high (thus, for $R = 1.2 \times 10^{-12}$ cm the value given in [8] is $Z_c = 200$, whereas exact calculation yields $Z_c = 170$). We note that at $Z \sim Z_c$ the electrostatic potential at the center of the nucleus reaches a value $V(0) = 3\zeta/2R \approx 60 m_e c^2$ at a nuclear radius $R \sim 0.03$ (in units $\hbar/m_e c = 3.86 \times 10^{-11}$ cm, i.e., $R = 1.2 \times 10^{-12}$ cm).

During the next stage, a more detailed investigation was made of the situation near $Z = Z_c$, when the lower electron level $1S_{1/2}$ merges with the continuum. Gershteĭn and Zel'dovich[9] proposed that when $Z > Z_c$ the bare nucleus Z emits spontaneously two positrons, after which the effective (renormalized, observable) charge of the bare nucleus decreases by two units, corresponding exactly to a filling of the K shell. The difference between the supercritical atom and the ordinary one lies in the fact that at $Z < Z_c$ these electrons should be taken from the outside. It is possible, for example, to produce two pairs $2e^- + 2e^+$ by photons having a frequency ω, after which the electrons land on the K shell, and the positrons go off to infinity. The pair-production threshold is equal to

$$\omega_{thr} = 1 + \epsilon_1, \qquad (1.2)$$

where ϵ_1 is the energy of the $1S_{1/2}$ level, i.e., pair production at $Z < Z_c$ calls for the expenditure of energy. At $Z = Z_c$ it is possible to produce a pair on a bare nucleus by a photon of arbitrary low frequency. At $Z > Z_c$, pair production is manifest as the production of positrons by the Coulomb field and the decrease of the nuclear charge proceeds spontaneously. According to the Pauli principle, only two electrons can be located at the 1S level, i.e., only two positrons will be emitted spontaneously, and it must not be assumed that the entire excess charge $(Z - Z_c)$ will be compensated or screened. However, in addition to the foregoing correct premises, Gershteĭn and Zel'dovich[9] made the erroneous statement that the wave function becomes delocalized when the state energy ϵ approaches the lower continuum.

Popov's investigations[10-12,65] of the Dirac equation at Z close to Z_c has cleared up the situation. Deferring the exact mathematical results to Secs. 2 and 4, we present here an intuitive interpretation of the phenomena at $Z \sim Z_c$. The Dirac equation for the electron has formal solutions also at negative $\epsilon < -1$ (the lower continuum). The properties of these solutions are determined by the fact that near $\epsilon = -1$, at distances $r > \hbar/m_e c$ from the nucleus, we deal in essence with positrons that are repelled from the positively-charged nucleus. The wave function has therefore a form characteristic of the nonrelativistic problem of a potential well with a Coulomb barrier.* It follows therefore that, owing to the barrier, the wave function is localized in the well (i.e., the distances from the nucleus are smaller than the Compton wavelength of the electron), and this localization is retained even as $Z \to Z_c$ ($\epsilon \to -1$), when the energy gap $\Delta = 1 + \epsilon$ between the bound state and the continuum tends to zero.

An analysis of the single-particle solutions of Dirac's equation leads to the following results. The discrete level 1S reaches the continuum boundary $\epsilon = -1$ at $Z = Z_c$ and then vanishes (at $Z > Z_c$, the discrete spectrum does not contain a solution that would continue the 1S level without interruption; the levels that follow the ground level, $2P_{1/2}$, $2S_{1/2}$, etc., are located at a finite distance from the continuum and have no singularity whatever at the point $Z = Z_c$). At $Z > Z_c$, however, a strong perturbation of the functions of the lower continuum $\psi_\epsilon(r)$ takes place and is due to the appearance of a pole in the scattering matrix at the point $E = \epsilon_0 - (i\gamma/2)(\epsilon_0 < 1)$. The perturbation of the functions $\psi_\epsilon(r)$ is concentrated mainly in the energy band $|\epsilon - \epsilon_0| \lesssim \gamma$, and in coordinate space it leads to the appearance of an additional charge density $\rho_0(r)$ of the vacuum. This density is localized at distances $r \approx \hbar/m_e c$ from the nucleus and carries a total charge $-2e$. In the region $(Z - Z_c) \ll Z_c$, the parameters ϵ_0 and γ depend on $Z - Z_c$ in the following manner:

$$\varepsilon_0 = -1 - a(Z - Z_c), \quad \gamma \sim \exp\left\{-b\sqrt{\frac{Z_c}{Z - Z_c}}\right\} \qquad (1.3)$$

where $a, b > 0$ are certain constants.†

When speaking of continuing the 1S level into the transcritical region, a distinction must be made between two possibilities. If this level is unfilled at the initial in-

*When we speak of a well with a barrier, we have in mind not the initial potential V(r) that enters directly in the Dirac equations (V(r) corresponds to attraction; e.g., $V(r) = -\zeta/r$), but a certain "effective" potential U(r). The latter arises when the system of the two Dirac equations (2.9) is reduced to a single second-order equation such as the Schrödinger equation. In the nonrelativistic case $U \approx V$; on the other hand, when $\epsilon \to -1$, the difference between the potentials U and V becomes quite significant. For details see Sec. 2 (particularly Fig. 2).

†The exponential smallness of γ is due to the small penetrability of the Coulomb barrier in the effective potential (2.15) for slow positrons.

stant of time (a bare nucleus with $Z > Z_c$ was produced somehow), then its continuation is the Breit-Wigner pole $E = \epsilon_0 - (i\gamma/2)$, i.e., the unfilled 1S level goes over into the quasiclassical state. Consequently, a bare nucleus with $Z > Z_c$ is unstable in vacuum. It can be stated that its Coulomb field produces in vacuum two electron-positron pairs, the electrons of which land on the K shell and the positrons go off to infinity after a time $t \gtrsim 1/\gamma$. The positron emission leaves a stable atom-like system ("supercritical atom") consisting of a nucleus Z plus the vacuum charge density $\rho_0(r)$ on the K shell. The charge distribution $\rho_0(r)$ is close in its physical properties (average radius etc.) to the charge density $\rho(r) = -e|\psi_0(r)|^2$ on the K shell in the ordinary atom with $Z < Z_c$, although the density $\rho_0(r)$ no longer corresponds to a single-particle wave function.

Unlike the ordinary nuclei, a bare nucleus with $Z > Z_c$ produces itself electrons that sit on the K shell.* On the other hand, if the K shell at $Z < Z_c$ is filled with electrons, then addition of several protons to the nucleus transfers the system directly to the supercritical state, and no positrons are emitted.†

The vacuum charge cloud $\rho_0(r)$ is a rather unusual object. First, the density $\rho_0(r)$ is localized in space ($\rho_0(r) \to 0$ as $r \to \infty$), but $\rho_0(r)$ does not coincide with the square of the single-particle wave function of the discrete spectrum, but is smeared out over the continuum (to be sure, when Z is only slightly larger than Z_c, the effective width of the energy band in the lower continuum, which contributes to the density $\rho_0(r)$, is of the order of γ, i.e., is exponentially small). Further, an atom with a supercritical charge (or the corresponding ion with a charge less than $Z - 2$), should have a curious singularity in positron scattering. When an external positron is scattered from such an atom, a narrow resonance is observed, and can be illustratively described as follows: The positron penetrates through the Coulomb barrier and experiences nonradiative annihilation with the electron located at the 1S "level." This results in a bare and unstable nucleus with a hole in the 1S shell; after a time $t \gtrsim 1/\gamma$ it produces spontaneously a positron and returns to the initial state. This process is analogous to excitation of an atom by a photon followed by spontaneous emission of a photon at the same frequency (within the limits of the line width γ). The positron scattering cross section is described by the Breit-Wigner formula. Independently of this illustrative description, the resonant scattering of positrons affords, in principle, a possibility of determining directly by experiment the parameters (real and imaginary parts of the energy $E = \epsilon_0 - (i\gamma/2)$, via the position and width of the resonance) of the quasistationary exponentially-decaying state which is a continuation of the discrete level at $Z > Z_c$.

It follows from the above-described properties of the electron cloud $\rho_0(r)$ that at $Z > Z_c$ we have in principle a many-body problem. This constitutes the third stage of the investigation of the $Z > Z_c$ situation, and has not been completed as yet. In an exact formulation, it is necessary to consider the equations of the electron-positron wave field with creation and annihilation operators, and to use the second-quantization formalism. The solutions of the one-electron problem (the Dirac equation in a specified external field V(r) are needed here as an intermediate step in the analysis of the entire many-particle problem. We have drawn physical conclusions above and we have predicted the results of real or hypothetical experiments on the basis of a consideration of single-particle solutions. In a rigorous approach such conclusions and predictions require a justification, which can be obtained only from the exact many-body theory. The expected change in the results consists of an additional shift of Z_c by an amount $\sim \alpha Z_c \approx 1$, which will henceforth be neglected.

Let us turn to more concrete aspects of our problem. The total spectrum of the single-particle states consist of a certain set of discrete levels with $-1 < \epsilon_n < 1$, an upper continuum $\epsilon > 1$, and a lower continuum $\epsilon < -1$. At any Z (both $Z < Z_c$ and $Z > Z_c$), the field of the nucleus deforms the wave functions of the continuum in a definite manner. The energy boundaries of the continuum ($\epsilon = \pm 1$) are naturally not altered thereby, since the potential of the nucleus at infinity is equal to zero.

It is well known that a change in the wave functions leads to a renormalization of the charge and to polarization of the vacuum. Let us refine these concepts.* The charge density of the vacuum contains a term $\rho' \propto \nabla^2\varphi$, i.e., proportional to the charge density ρ_{ext} of the nucleus producing the potential: $\rho'(r) = (1/4\pi) \times (1 - Z_3^{1/3})\nabla^2\varphi$ (or, in the momentum representation, $\rho'_k \sim k^2\varphi_k$). This term is eliminated by introducing the renormalized charge density

$$\rho_R = \rho_{ext} + \rho' = Z_3^{1/2}\rho_{ext} \tag{1.4}$$

and substituting subsequently in the equations $\rho_R(r)$ for $\rho_{ext}(r)$. Experiment yields precisely $\int \rho_R\, dV$, or the charge corresponding to one or several protons. On the other hand, the quantities $\rho_{ext}(r)$ and Z_3 are unobservable and drop out from a comparison of the theory with experiment. This is fortunate, since Z_3 is expressed by a diverging integral.† The renormalizability of electrodynamics indeed consists in the fact that the comparison of theory with experiment turns out to be independent of the cut-off parameter Λ when $\Lambda \gg m_e$.

However, even in the first perturbation-theory order in φ, there are terms of higher order in the wave vector k (in the linear theory it is convenient to use the Fourier expansion of the potential):

$$\rho''_k = \frac{\alpha}{4\pi^2}\left\{\frac{k^4}{15m_e^2}\varphi_k + \frac{k^6}{170m_e^4}\varphi_k + \ldots\right\} \tag{1.5}$$

*As follows from (1.3) the time of transformation of a bare nucleus with $Z > Z_c$ into a supercritical atom depends exponentially on $Z - Z_c$ and is large compared with the time $\hbar/m_ec^2 = 1.3 \times 10^{-21}$ sec which is characteristic of electrodynamics (at least so long as $Z - Z_c \ll Z_c$).

†Of course, the total charge of the supercritical atom need not necessarily remain equal to Z−2. Electrons coming from the outside can fill the next shells (with level energies $\epsilon > -1$), thereby decreasing the charge further, producing even a neutral atom. In this respect there is no difference from the filling of the shells in an ordinary atom with $Z < Z_c$.

*We do not pretend to make any general formulations below, and consider only the static case $A = 0$, with $A_0 = \varphi(r)$ independent of t.

†The divergent part of the induced charge density $\rho'(r)$ is exactly proportional to the external charge $\rho_{ext}(r)$. Consequently the renormalization procedure completely eliminates the divergences from the theory.

or

$$\rho''(\mathbf{r}) = \frac{\alpha}{\pi}\left\{-\frac{1}{15m_e^2}\Delta\rho_R + \frac{1}{170m_e^4}\Delta\Delta\rho_R + \ldots\right\} \qquad (1.5')$$

(see, e.g., [13]; here $\alpha = e^2/\hbar c = 1/137$). Besides $\rho'(\mathbf{r})$, an additional charge density, which does not reduce to a renormalization of the charge, arises in the electron-positron vacuum perturbed by the external field. The quantity $\rho''(\mathbf{r})$ is customarily called the polarization of vacuum.

Let us note the general properties of $\rho''(\mathbf{r})$. First, $\int \rho'' dV = 0$, since the integral over the entire volume corresponds to the Fourier component of ρ_k'' with $k = 0$, and the expansion (1.5) begins with k^4 (if we start from φ) or with k^2 (if we start from ρ_R). Thus, the polarization of vacuum does not change the total charge (and the field at infinity). So long as we stay within the framework of the linear theory, we can assume this to be a consequence of the definition of the renormalized charge, i.e., of the foregoing subdivision of the effect into charge renormalization and vacuum polarization. We note further that if we confine ourselves to expansion of ρ_k'' in powers of k^2, then the charge density $\rho''(\mathbf{r})$ differs from zero only where $\rho_R(\mathbf{r}) \neq 0$. Actually, however, the complete expression for ρ_k'' is not described by the series, since it does not converge at $|k^2| > 4m_e^2$. Related to this mathematical circumstance is the fact that $\rho''(\mathbf{r})$ differs from zero also in the region where $\rho_{ext}(\mathbf{r}) = 0$. In particular, even in the approximation linear in Z the charge density induced in vacuum by a point-like charge differs from zero (see Sec. 4 below). As is well known, the first term $\sim k^4\varphi_k$ in (1.5) makes a contribution of -27 MHz to the Lamb level shift, as is fully confirmed by experiment.

The polarization of vacuum in the general case should also contain terms of higher order in the potential $\varphi(\mathbf{r})$ or in the electric field. They could be ignored in the initial theory of the Lamb shift in the hydrogen atom, but we are interested in the case of nuclei with large charges, where the expansion parameter $\zeta = Z\alpha$ is of the order of unity. The calculations of the polarization of vacuum in higher orders in the parameter ζ becomes unusually difficult and cumbersome (they were carried out up to ζ^3; see [15]). Experiment shows that in this case the polarization of vacuum likewise does not change the total charge.*

The question arises of how to verify that the theory actually agrees with experiment in the most important prediction $\int \rho''(\mathbf{r})dV = 0$. The analogy with dielectrics can be useful here. The main similarity between these problems lies in the fact that the dielectric, like the vacuum, has a gap between two continua.†

Besides the charge density ρ'', we introduce the charge displacement $\mathbf{P}$: $\rho'' = -\operatorname{div}\mathbf{P}$ (we shall not use here the term "polarization," to avoid confusion with the polarization of vacuum). In a weak and slowly varying field in a dielectric we have $\mathbf{P} = f\mathbf{E}$, where the constant f is connected with the dielectric constant: $\epsilon = 1 + 4\pi f$. In a strong field $\mathbf{P} = f(E^2)\mathbf{E}$, and f is no longer a constant independent of the field. However, owing to the divergent connection between ρ'' and $\mathbf{P}$, the change of f makes no contribution to $\int \rho'' dV$, since this integral is identically equal to the limit

$$\lim_{R\to\infty} 4\pi R^2 P(R) = \lim_{R\to\infty} 4\pi R^2 f(E^2) E = 0. \qquad (1.6)$$

In exactly the same way, the dispersion, namely the dependence of the function f on the wave vector $\mathbf{k}$, makes no contribution. The total change of the charge is determined by one number—the static dielectric constant, or more accurately by the limiting value of f as $E^2 \to 0$ and $k^2 \to 0$. In other words, all that matters is the displacement $\mathbf{P}$ far away (in the limit as $r \to \infty$), where the field $\mathbf{E}$ is small and is almost constant.

The situation is apparently similar for the polarization of vacuum, the only difference being that the "dielectric constant" of vacuum is included in the renormalization concept. It seems to us that there has never been a complete analysis of the polarization of vacuum outside the framework of perturbation theory,* although there is no doubt of the final result.

The known results pertaining to the case $Z < Z_c$ were described above perhaps too pedantically, in order to explain better the features of the new situation arising when $Z > Z_c$. In this case, after the lower level 1S merges with the continuum (at $Z = Z_c$), a quasistationary state with complex energy $E = \epsilon_0 - (i\gamma/2)$ is produced in the single-particle problem ($\epsilon_0 < -1$). Although such solutions do not enter in the new set of orthonormalized solutions of the Dirac equation (in the "spectrum" of this equation), their existence does not fail to affect the functions of the continuous spectrum. At the real energy ϵ close to the pole (i.e., at $|\epsilon - \epsilon_0| \lesssim \gamma$), the wave functions of the continuous spectrum experience characteristic changes, namely: at a given normalization at infinity ($\chi_k(\mathbf{r}) \approx \sqrt{2/\pi}\sin(kr + \delta)$), a strong increase takes place in $\chi_k^2(0) \sim \gamma[(\epsilon - \epsilon_0)^2 + (\gamma^2/4)]^{-1}$.

Thus, an additional term appears in the integral of the charge density over the continuous spectrum. The localization of this term follows the intrabarrier density $\chi_0^2(\mathbf{r})$ of the quasistationary state. It is this additional charge density which corresponds effectively to two bound electrons. A formal proof of this statement will be given in Sec. 4.

The analysis of the relativistic case is made complicated by integration over infinite momentum space. How-

*L. P. Pitaevskiĭ has correctly remarked that we can get along here without reference to experiment; the fact that the renormalization is independent of the charge is a profound property of the theory, connected with charge conservation and gauge invariance. When considering a hypothetical experiment of "assembling" a lead nucleus consisting of 82 protons and 126 neutrons, gauge invariance leads to the result that the field at infinity remains unchanged. A change by an integer times e is possible if real electrons or positrons go off to infinity.

†The roles of the upper and lower continua are played here by the valence and conduction bands. Deep levels in semiconductors are customarily defined as those whose binding energy is comparable with the distance between the bands (such levels are produced near multiply-charged impurity centers, vacancies, etc., and play an important role in semiconductor physics). The theory of deep levels is reminiscent in many respects of the relativistic problem with a potential (see the paper by Keldysh [16]).

*With the exception of the simplest case of fields E and H that are homogeneous in space and constant in time [17,18] (see also the recent paper [19]).

ever, the region $p \gg m_e c$ actually does not contain a specific dependence on $Z - Z_c$, and therefore its contribution vanishes after the renormalization. An important fact for the entire analysis is that the sum of the squares of the wave functions

$$\rho(r) = \sum_n \psi_n^2(r) + \int dk\, |\psi_k(r)|^2 \qquad (1.7)$$

(over the discrete levels and the continuum) experiences no singularity whatever (e.g., a discontinuity in $\rho(r)$ or in its derivative) at the instant when a discrete-spectrum level appears or vanishes while the depth of the potential is smoothly varied (see [20] and also [21-24]).

We apply these considerations to nuclei with large Z. When $Z < Z_c$ there is a discrete level $1S_{1/2}$ above the continuum. If it is filled with electrons, then there is no doubt that the charge of the system is $Z - 2$. For the reasons stated above, this quantity cannot change on going through $Z = Z_c$. The difference between the cases $Z > Z_c$ and $Z < Z_c$ is that when $Z < Z_c$ the density of the electron cloud is equal to $\rho_0(r) = -e\psi_0^2(r)$, where $\psi_0(r)$ is the wave function of the lower level, and when $Z > Z_c$ this density does not correspond to any wave function of the single-particle approximation (the K-shell wave function becomes a multi-particle one). The density $\rho_0(r)$ at $Z > Z_c$ is a perturbation of the wave functions of the lower continuum $\psi_\epsilon(r)$, concentrated in a narrow band $|\epsilon - \epsilon_0| \sim \gamma$.

The spatial dependence of $\rho_0(r)$ does not experience any sharp changes at the point $Z = Z_c$.

So long as the level $1S_{1/2}$ has not yet merged with the lower continuum, the wave functions of the continuum $\chi_\epsilon(r)$ are orthogonal to the function $\chi_0(r)$. After the merging, the wave functions $\chi_\epsilon(r)$ in the vicinity of the resonance ($|\epsilon - \epsilon_0| \lesssim \gamma$) are similar to $\chi_0(r)$, if r is not too large (under the barrier).

It is important, of course, that we are dealing here with fermions and that the Pauli principle holds. Light charged bosons (if such were to exist in nature), taken in place of electrons, could be produced virtually in arbitrary amounts and could screen spontaneously the entire excess charge $Z - Z_c$ (this question was considered in detail recently by A. B. Migdal[25]). On the other hand, electrons, as a result of the Pauli principle, screen only two charge units. Therefore the picture of the phenomena at $Z > 170$, obtained in the single-particle approximation, remains valid also in the multi-particle problem (the greatest change introduced by the multi-particle analysis may cause the statement made above for a certain Z to turn out to be valid also for a nucleus with charge $Z' = Z + \Delta Z$, where $\Delta Z \sim \alpha Z_c \sim 1$).

This is the general picture of the phenomena at $Z \sim Z_c$. Let us make a few remarks concerning the accuracy of the calculations of Z_c.

At $Z < Z_c$, allowance for the vacuum polarization makes the potential well deeper (the corresponding level shift $\Delta E''$ is always negative, and for hydrogen it makes a contribution -27 MHz to the radiative shift of the levels $2S_{1/2}$ and $2P_{1/2}$). Therefore the polarization of the vacuum decreases the value of Z_c by an amount $\sim \alpha Z_c$.

On the other hand, allowance for the electronic self-energy diagrams (interaction of electron with photon vacuum) raises the level. The calculation of this part of the Lamb shift (which we denote by $\Delta E'$) for heavy atoms is the subject of [26-29]. At $Z\alpha \ll 1$ the following estimate is valid[30,31]

$$\Delta E'_{nl} \approx \frac{4\alpha}{3\pi} \delta_{l0} \frac{(Z\alpha)^4}{n^3} \ln \frac{1}{(Z\alpha)^2}. \qquad (1.8)$$

At $Z\alpha \sim 1$ we should expect $\Delta E'_{ne} \sim \alpha m_e c^2$, i.e., the radiative shifts can change Z_c by an amount on the order of αZ_c.

Let us list the main conclusions concerning the behavior of atoms and nuclei with large Z:

1) At $Z > Z_c$ a bare nucleus, after emitting two positrons, surrounds itself by the K shell and is transformed into a supercritical atom. Its charge, determined from the electrostatic field at distances $r > \hbar/m_e c$, is equal to $Z - 2$.

2) A characteristic feature of this problem is the existence of a Coulomb barrier for an electron with negative energy $\epsilon \approx -1$. Because of this barrier, the wave function at $Z = Z_c$ does not become localized, the discrete level 1S in the bare nucleus has a continuation in the form of a resonance $E = \epsilon_0 - i\gamma/2$, and the probability of emission of positrons at $Z > Z_c$ vanishes exponentially at the threshold.

3) When the charge of the nucleus is raised to $Z > Z_c$, an atom with a filled K shell goes over directly into the supercritical state, without emitting positrons.

4) The properties of the outer shells of the atom (which determine, in particular, the Mendeleev periodicity of the chemical properties) continue in regular fashion into the transcritical region.

There is a certain analogy between positron production by a nucleus at $Z > Z_c$ and pair production in a homogeneous electrostatic field.

The interaction of an electromagnetic field with a vacuum of charged particles leads to the appearance of nonlinear increments to the Lagrangian of the electromagnetic field L,[32,33] and pair production is only one aspect of the phenomena connected with these nonlinearities. Namely, the probability w of pair production by an external field is determined by Im L (see [17]). In the case of fields E and H that are constant (in time and in space), an exact solution of the problem is possible; it was obtained by Schwinger[17] for scalar and spinor electrodynamics and in [18] for charged vector bosons with a gyromagnetic ratio $g = 2$. In particular, the following expression was obtained in these papers for the pair-production probability in a constant electric field E:

$$w = 2\,\mathrm{Im}\,L = (2s+1)\frac{m^4}{2\pi^2}\left(\frac{E}{E_c}\right)^2 \sum_{n=1}^{\infty} \frac{\beta_n}{n^2} \exp\left(-\frac{n\pi m^2}{eE}\right) \qquad (1.9)$$

(see also [34]). Here $\hbar = c = 1$, s and m are the spin and mass of the particles produced by the field E, $\beta_n = (-1)^{n-1}$ for bosons and $\beta_n = 1$ for fermions; the probability w is measured in units of $m^4c^5/\hbar^4$ (which corresponds to the number of pairs produced in the volume $(\hbar/mc)^3$ after a time $\hbar/mc^2$). The argument of the exponential in (1.9) is of the form $n\pi E_c/E$, where $E_c = m^2c^3/e\hbar = 1.3 \times 10^{16}$ V/cm for electrons (since $E_c \sim m^2$, the characteristic intensity E_c for other charged particles is even larger). So long as $E < E_c$, the probability w is exponentially small and its suffices to retain in the sum (1.9) the first

term with n = 1, corresponding to the quasiclassical approximation.*

Pair production ceases to be a small effect at $E \sim E_c$. We note now that in the Coulomb field of the nucleus Z the intensity $E = Ze/r^2$ is comparable with E_c when $r \sim r_c = \zeta^{1/2}\hbar/mc$, with $|V(r_c)| = \zeta^{1/2}mc^2$. At $m = m_e$ and $\zeta > 1$, there is a region $r \lesssim r_c$ near the nucleus, in which pair production is possible (in this case the static field must satisfy the condition $|V(r)| > 2m_ec^2$), after which the electron is bound to the nucleus, and the positron goes off to infinity through the Coulomb barrier. This intuitive (albeit not rigorous) reasoning establishes the connection between the phenomena in the Coulomb field at $Z > Z_c$ and the Schwinger formula (1.9). Of course, one cannot expect here literal coincidence of the formulas for the probability w, since (1.9) is valid only for a homogeneous field, and the Coulomb field is strongly inhomogeneous at small distances.

In concluding the introductory "bibliographic" part of the review, we wish to say a few words concerning the estimate of the position occupied by this phenomenon in science. Views are sometimes expressed, that sciences can be classified in accordance with the scale of the phenomena investigated in them. In this case, priority goes immediately to the astronomers, who study explosions of stars, bursts of quasars, and the "big-bang" expansion of the universe as a whole.

The progress in astrophysics, however, would be impossible without the development of the theory of elementary particles, which is of tremendous cognitive significance, and furthermore, without explaining the fundamental processes in this theory it is impossible to make progress also in other branches of science. There is no doubt that a clear and thorough understanding of all the details of polarization of vacuum and pair production is a necessary albeit partial stage in the development of the theory of elementary particles.

It is curious that the correct answer to the question of the significance of the theory of the structure of matter was given half a century ago by Russian poets.

Recently, it became fashionable to contrast physicists and lyricists. That the artist has lost close contact with scientific progress is clearly evident. Yet at one time, in the 20's the theory of relativity and the structure of the atom have greatly inspired the imagination of all thinking persons. Valeriĭ Bryusov in metered verse drew a picture of the planetary system of the atom,[37] anticipating certain modern ideas concerning the structure of particles. But an even more remarkable awareness of the close connection between the theory of the microworld and the cosmos is expressed in a two-line poem of Velemir Khlebnikov:

> The host of heaven is far, powerful, and mighty,
> but to understand it, know the atom's constitution.†

2. LEVELS OF SINGLE-PARTICLE DIRAC EQUATION

2.1. As is well known,[5,13] the Dirac equation for an electron in the Coulomb field of a point-like charge Ze can be solved exactly, and the level energies are equal to

$$\varepsilon_{nj} = \left[1 + \frac{\zeta^2}{(n - |\varkappa| + \sqrt{\varkappa^2 - \zeta^2})^2}\right]^{-1/2}; \qquad (2.1)$$

here $\zeta = Z\alpha = Z/137$, n is the principal quantum number ($n = 1, 2, 3, \ldots$) and $-\kappa$ is the eigenvalue of the Dirac operator $K = \beta(1 \cdot \sigma + 1)$, which is the integral of motion in any field with spherical symmetry:*

$$\varkappa = \mp(j + 1/2) \quad \text{for} \quad j = l \pm 1/2. \qquad (2.2)$$

For light atoms, formula (2.1) can be expanded in powers of ζ^2:

$$E_{nj} = \varepsilon_{nj} - 1 = -\frac{\zeta^2}{2n^2}\left[1 + \frac{\zeta^2}{n}\left(\frac{1}{|\varkappa|} - \frac{3}{4n}\right)\right]. \qquad (2.3)$$

In the nonrelativistic approximation ($\zeta \ll 1$), E_{nj} does not depend on j and (2.3) goes over into the ordinary expression for the spectrum of the hydrogen atom: $E_n = -\zeta^2/2n^2$. The level E_n has here a degeneracy multiplicity $2n^2$ ($j = \frac{1}{2}, \frac{3}{2}, \ldots, (n-1)/2$, and the number κ assumes values $\kappa = \pm 1, \pm 2, \ldots, \pm(n-1), -n$).

We shall be interested, however, in the opposite case of large Z, when $\zeta \sim 1$. Formula (2.1) remains meaningful so long as $\zeta < |\kappa| = j + \frac{1}{2}$. As $\zeta \to |\kappa|$, it acquires a root singularity

$$\varepsilon_{nj} = \frac{n - |\varkappa|}{N} + \frac{\varkappa^2}{N^3}\sqrt{\varkappa^2 - \zeta^2} + \ldots, \qquad (2.4)$$

where $N = \sqrt{n^2 - 2|\kappa|n + 2\kappa^2}$, $n \geq |\kappa|$. Further continuation of (2.1) into the region $\zeta > |\kappa|$ causes the energy ϵ_{nj} to become complex, which is physically meaningless (for the states of the discrete spectrum in the single-electron problem!).

This difficulty is explained by the fact that the effective potential U(r), which arises when the Dirac equation is squared, behaves for a Coulomb field $V(r) = -\zeta/r$ as $r \to 0$ in a singular manner: $U(r) \approx (j(j+1) - \zeta^2)r^{-2}$, i.e., the so-called "falling to the center" appears when $\zeta > j + \frac{1}{2}$.[38-40] In this case, to determine the level energies, it does not suffice to specify the potential V(r) at $0 < r < \infty$, but it is also necessary to impose a boundary condition at zero; only then does the problem become mathematically correct (for details see [38,40].)

2.2. The assumption that the Coulomb potential becomes infinite at r = 0 is an idealization. Actually, for various reasons (finite dimensions of the nucleus, polarization of vacuum, etc.), the formula $V(r) = -\zeta/r$ becomes modified in some manner or another when $r \to 0$. However, so long as $\zeta < j + \frac{1}{2}$, the level energy ϵ depends little on the concrete form of V(r) at small r, and it is therefore permissible to go to the limit of a point Coulomb field. On the other hand, if $\zeta \geq j + \frac{1}{2}$,

*In this case it is possible to develop a quasiclassical method of calculating w, connected with the calculation of the action S along the sub-barrier trajectories with imaginary time [35]. This method is effective for a large class of time-variable fields. For certain fields of special form, an exact solution of the Dirac equation was recently obtained and exact formulas were derived for the probability w [19,36].

†Researches by Ya. B. Zel'dovich.

*We recall that for a relativistic electron in a field V(r), only the total angular momentum $j = l + \sigma/2$ is conserved, and the orbital angular momentum l has no definite value. By l and l' we shall denote the orbital angular momenta corresponding to the upper and lower components of the Dirac bispinor ($l + l' = 2j$). States having the same j but different signs of κ have different parity [13,14].

then the dependence of ϵ on the type of cutoff of V(r) becomes significant, a feature characteristic of all problems with "falling to the center."

In the region $\zeta \approx j + \frac{1}{2}$ it is necessary to cut off the potential of the point-like charge and make it finite at zero:

$$V(r) = \begin{cases} -\zeta/r & \text{for } r > R, \\ -\frac{\zeta}{R} f\left(\frac{r}{R}\right) & \text{for } 0 < r < R. \end{cases} \quad (2.5)$$

From the mathematical point of view, such a procedure is a regularization that makes the problem unique, and from the physical point it takes into account the finite dimensions of the nuclei.

The form of the cutoff function at f(x) depends on the distribution of the electric charge over the volume of the nucleus ($x = r/R$, $0 < x < 1$, with $f(1) = 1$). Thus, $f(x) = (3 - x^2)/2$ corresponds to a constant volume density of the charge, and the simplest choice $f(x) \equiv 1$ corresponds to concentrating the entire charge on the surface of the nucleus.

Such a formulation of the problem is due to Pomeranchuk and Smorodinskiĭ,[8] who gave a (qualitatively) correct description of the phenomena at $Z \approx 137$, namely, with increasing Z the levels continue to drop, until the lower level of the discrete spectrum $1S_{1/2}$ reaches the boundary $\epsilon = -1$ at a certain "critical" $Z = Z_c > 137$.

We shall show first that any cutoff of the potential V(r) eliminates singularities of the type (1.1) at the energies ϵ_{nj}, and that the curve of the level $\epsilon = \epsilon(\zeta)$ continues smoothly to $\epsilon = -1$.

This property of the solutions of the Dirac equation is valid not only for the potential (2.5), but also in the general case. Indeed, let us consider an arbitrary attraction potential $V(r) = -\zeta v(r)$, where $v(r) \geq 0$ is a fixed function of r, and let us vary the coupling constant ζ. With respect to v(r) we assume, first, that it is bounded, i.e., $\max_{0 \leq r < \infty} v(r) < C$, where C is assumed constant, and second that $v(r) \to 0$ as $r \to \infty$. Assume that at a certain value of ζ there is a bound level with energy ϵ and wave functions $G = G(r; \zeta)$ and $F = F(r; \zeta)$. Here and below $G = rg(r)$ and $F = rf(r)$, while g(r) and f(r) are radial functions for the upper and lower bispinor components defined in accordance with [13]. The normalization condition is

$$\int_0^\infty (G^2 + F^2)\, dr = \int_0^\infty (g^2 + f^2)\, r^2 dr = 1. \quad (2.6)$$

After calculating by perturbation theory the change of the level energy following an infinitesimally small deepening of the well, we get

$$\frac{\partial \varepsilon}{\partial \zeta} = -\int_0^\infty v(r)\,(G^2 + F^2)\, dr \quad (2.7)$$

(this formula is exact if G and F are the exact wave functions of the level with energy ϵ). Since $0 \leq v(r) < C$, we get

$$-C < \frac{\partial \varepsilon}{\partial \zeta} < 0. \quad (2.8)$$

This means that any level drops monotonically with increasing coupling constant ζ, and the $\epsilon = \epsilon(\zeta)$ curve has no singularities (the derivative $\partial\epsilon/\partial\zeta$ is finite everywhere). Consequently, it cannot be cut off (like (1.1) or (2.1)) without reaching the limit $\epsilon = -1$ of the lower continuum.*

We note that the situation is not so simple for other relativistic wave equations (with the exception of the Dirac equation)—see Sec. 5.

2.3. We proceed to a more detailed study of the behavior of the level and of the properties of the wave functions near $\epsilon = -1$. To this end, it is convenient to reduce the system of equations for the functions G and F

$$\frac{dG}{dr} = -\frac{\varkappa}{r} G + (1 + \varepsilon - V) F, \quad \frac{dF}{dr} = (1 - \varepsilon + V) G + \frac{\varkappa}{r} F \quad (2.9)$$

to a single second-order equation having formally the same form as the nonrelativistic Schrödinger equation (with a certain effective potential). To this end we eliminate from (2.9) the function F:

$$G'' + \frac{V'}{1 + \varepsilon - V}\left(G' + \frac{\varkappa}{r} G\right) + \left[(\varepsilon - V)^2 - 1 - \frac{\varkappa(\varkappa+1)}{r^2}\right] G = 0, \quad (2.10)$$

and then, using the substitution $G(r) = [1 + \epsilon - V(r)]^{1/2} \times \chi(r)$, we reduce (2.10) to the self-adjoint form

$$\chi'' + k^2(r)\,\chi = 0; \quad (2.11)$$

here $k^2(r) = 2(E - U)$, $E = (\epsilon^2 - 1)/2$, and it is convenient to break up the effective potential U(r) into two parts, $U = U_1 + U_2$, where U_1 coincides with the effective potential in the Klein-Gordon equation†

$$U_1 = \varepsilon V - \frac{1}{2} V^2 + \frac{\varkappa(\varkappa+1)}{2r^2}, \quad (2.12)$$

and U_2 is due to spin effects:

$$U_2 = \frac{1}{4}\left\{\frac{V''}{1 + \varepsilon - V} + \frac{3}{2}\left(\frac{V'}{1 + \varepsilon - V}\right)^2 - \frac{2\varkappa V'}{r(1 + \varepsilon - V)}\right\}. \quad (2.13)$$

This expression becomes much simpler at $\epsilon = -1$. For a qualitative analysis we can confine ourselves to this case, for when ϵ is close to -1 the dependence of U_2 on ϵ is weak (for an attraction potential $V(r) \leq 0$ the denominator $1 + \epsilon - V$ never vanishes, so that we can go through the boundary $\epsilon = -1$). We put also $\kappa = -1$, corresponding to the ground state (in this case the centrifugal barrier in $U_1(r)$ vanishes). Then ($\epsilon = \kappa = -1$)

$$U_1 = \frac{1}{2}[1 - (1 + V)^2], \quad U_2 = -\frac{u^2 - u'}{2} + \frac{\varkappa u}{r}, \quad (2.14)$$

where $u(r) = V'/2V$ (the potentials U and V are measured in units of $m_e c^2$). At small distances, the relativistic term $-V^2/2$ predominates in $U_1(r)$ and leads to attraction (regardless of the sign of the initial potential V). On the other hand, as $r \to \infty$ we have $U_1(r) \approx \epsilon V(r)$, i.e., the sign of the "tail" of the effective potential is itself dependent on the sign of ϵ. In particular, if $V(r) < 0$ and $\epsilon < 0$, then $U_1(r)$ at large distances corresponds to repulsion. It is seen from (2.14) that U_1 has a maximum of height $m_e c^2/2$ at the same point $r = r'_m$ where

*In the case of a point-like charge we have, in accordance with (1.1), $\partial\epsilon_1/\partial\zeta = -\infty$ at $\zeta = 1$. This also agrees with (2.7) if it is recognized that here $v(r) = r^{-1}$, and the functions G and F at $\zeta = 1$ are finite at zero (for the ground state at $\zeta = 1$ we have $g = -f = e^{-r}/r$, i.e., the radial functions g(r) and f(r) become singular at the point r = 0). Any cutoff of the potential $V(r) = -\zeta/r$ as $r \to 0$ eliminates this singularity and makes $\partial\epsilon_1/\partial\zeta$ finite.

†We note that $\kappa(\kappa + 1) = l(l + 1)$, i.e., $U_1(r)$ includes the centrifugal energy $l(l + 1)/2r^2$. It is important that in the nonrelativistic problem (2.11) the values $\epsilon \approx -1$ correspond to energies E close to zero.

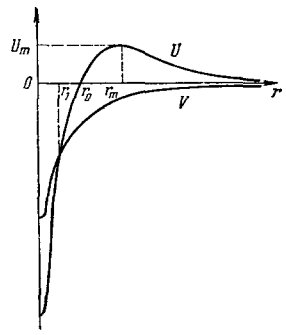

FIG. 2. The potential V(r) and the effective potential U(r) for the Coulomb problem at $Z \to Z_c$ and $\epsilon = -1$.

$V(r_m') = -1$, and that at $V(r_0') = -2$ we have $U_1(r_0') = 0$. We arrive at the conclusion that at $\epsilon \approx -1$, in an effective potential U(r), unlike in V(r), there is a sufficiently high potential barrier. This conclusion remains the same also if the spin term U_2 is taken into account. Thus, in the case of a Coulomb field $V(r) = -\zeta/r$ we obtain

$$U(r) = U_1 + U_2 = \frac{\zeta}{r} - \frac{\eta}{2r^2}, \qquad (2.15)$$

where $\eta = \zeta^2 - \kappa^2 + (1/4)$. To obtain more accurate results at small r, we add to U(r) also the term $1/8r^2$ (this is a correction well known from the quasiclassical theory,[39] due to Langer[41,42], and reduces to a replacement of $j(j+1)$ by $(j+\frac{1}{2})^2$), after which we have $\eta = \zeta^2 - \kappa^2$. The connection between the potentials V and U is shown in Fig. 2. At the point where U(r) has a maximum we have

$$r = r_m = \frac{\zeta^2 - \kappa^2}{\zeta}, \quad U_{\max} = \frac{\zeta^2}{2(\zeta^2 - \kappa^2)} > \frac{1}{2} \quad (\text{for } \zeta > \kappa). \qquad (2.16)$$

Other characteristic points (see Fig. 2) are $r_0 = r_m/2$ and $r_1 = r_m/4$. In the region $r < r_1$ we have $U < V$, i.e., the effective potential U(r) corresponds to a deeper well than V(r). For $\kappa = -1$ (ground state) and $\zeta = 1.25$ (the real value of ζ_c for a nucleus with radius $R \sim 10^{-12}$ cm) we obtain $r_m = 0.45\hbar/m_e c \approx 1.7 \times 10^{-11}$ cm and $U_{\max} = 1.4 m_e c^2$.

Thus, for an electron in a state with energy $\epsilon \approx -1$ there is a broad Coulomb barrier, the penetrability of which is exponentially small as $\epsilon \to -1$. This circumstance is important for everything that follows. The wave function with energy ϵ has an asymptotic form ($r \to \infty$)

$$G(r) \approx A\sqrt{1+\varepsilon}\, e^{-\lambda r} r^{\epsilon\zeta/\lambda},$$
$$F(r) \approx -A\sqrt{1-\varepsilon}\, e^{-\lambda r} r^{\epsilon\zeta/\lambda} \qquad (2.17)$$

($\lambda = \sqrt{1-\epsilon^2}$; the constant A is determined from the normalization). The factor $r^{\epsilon\zeta/\lambda}$ is due to the Coulomb interaction of the electron with the nucleus, which greatly distorts the wave function at large distances. As $\epsilon \to +1$ there is no barrier in U(r), $\epsilon\zeta/\lambda \to +\infty$, and the maximum $G^2(r) + F^2(r)$ goes off to large distances—delocalization of the bound state takes place. Such a behavior of the states adjacent to the edge of the continuous spectrum is well known from nonrelativistic quantum mechanics.* As $\epsilon \to -1$, an entirely different picture is produced, namely, $\epsilon\zeta/\lambda \to -\infty$, the factor $r^{\epsilon\zeta/\lambda}$ decreases more rapidly than any finite power of r, and the electron remains localized near the nucleus. The asymptotic form of the wave functions in the case $\epsilon = -1$ can be obtained from the following considerations. If $U(r) = \zeta/r$ as $r \to \infty$ (with $\zeta > 0$), then the Schrödinger equation has a solution that decreases at infinity, in the form

$$\chi(r) \sim r^{1/4} e^{-\sqrt{8\zeta r}}. \qquad (2.18)$$

On the other hand, to change over from the system (2.9) to the Schrödinger equation (2.11) in the case $\epsilon = -1$ it is necessary to make the substitution

$$G(r) = \sqrt{V(r)}\,\chi_1(r), \quad F(r) = \sqrt{2+V(r)}\,\chi_2(r).$$

It follows therefore that for $\epsilon = -1$ and $r \to \infty$

$$G(r) = A'\left(\frac{2r}{\zeta}\right)^{-1/4} e^{-\sqrt{8\zeta r}}, \quad F(r) = -A'\left(\frac{2r}{\zeta}\right)^{1/4} e^{-\sqrt{8\zeta r}}. \qquad (2.19)$$

We call attention to the behavior of the wave functions, namely, G, $F \propto \exp(-\sqrt{8\zeta r})$. This decrease of G and F is none other than the damping under the Coulomb barrier. We emphasize the difference between the asymptotic form of (2.19) and the usual exponential $\chi \propto e^{-\lambda r}$ which is valid for the indicated states in the short-range potential (here $\lambda = \sqrt{-2E}$). In the latter case, at $E \to 0$, delocalization is inevitable, whereas in our problem, owing to the Coulomb barrier in U(r) the wave functions at $\epsilon = -1$ attenuate at infinity, although in this case $E = (\epsilon^2 - 1)/2 = 0$ and $\lambda = 0$.

On the boundary of the upper continuum ($\epsilon = +1$) the asymptotic behavior of the two functions is as follows:

$$G(r) \approx A''\left(\frac{2r}{\zeta}\right)^{1/4} \sin(\sqrt{8\zeta r} + \delta),$$
$$F(r) \approx A''\left(\frac{2r}{\zeta}\right)^{-1/4} \cos(\sqrt{8\zeta r} + \delta). \qquad (2.20)$$

By virtue of the continuity it is clear that in the continuous spectrum the functions with energy $\pm\epsilon$ should differ strongly from one another, particularly as $|\epsilon| \to 1$. In the quasiclassical approximation

$$G,\ F \sim \exp\left(\pm i \int^r p\, dr\right), \text{ where } p(r) = \sqrt{\epsilon^2 - 1 + \frac{2\epsilon\zeta}{r} + \frac{\zeta^2 - 1}{r^2}}. \qquad (2.21)$$

When $\epsilon > 1$, we have $p^2(r) > 0$ and the functions G and F oscillate at all r. On the other hand, if $\epsilon < -1$, then there is a turning point $r_n = 2|\epsilon|\zeta/(\epsilon^2 - 1)$, which lies far from the nucleus at values of ϵ close to -1. In the classically-forbidden region $r < r_n$ the wave functions contain, generally speaking, two exponentials $\exp(\pm\sqrt{8\zeta r})$, and the oscillations* described are the asymptotic formula (2.17) set in only at $r > r_n$. An approximate form of the wave functions near $\epsilon = -1$ is shown in Fig. 3.

2.4. Having explained the quantitative aspects, we now proceed to an exact solution of the problem. We confine ourselves to a presentation of the main formulas, and refer the reader to [10-12] for mathematical details.

In a field $V(r) = -\zeta/r$, Eqs. (2.9) for the functions G and F can be solved exactly. The solution has a particularly simple form at $\epsilon = -1$:

$$G(r) = K_{i\nu}(\sqrt{8\zeta r}), \quad F(r) = \frac{1}{\zeta}(rG' + \kappa G); \qquad (2.22)$$

*For example, for a hydrogen atom in a state with principal quantum number n we have $\chi_{nl}(r) \sim e^{-r/n} r^n$ as $r \to \infty$, i.e., the average radius is $\bar{r} \sim n^2$.

*When $\epsilon < -1$ we have $\lambda = \pm ip = \pm i\sqrt{\epsilon^2 - 1}$ and formula (2.17) takes the form $G, F \sim \exp\{\pm i(pr + \epsilon\zeta/p \ln 2pr)\}$.

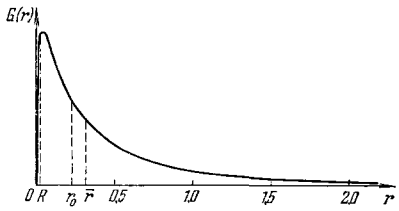

FIG. 3. The wave function G(r) at $\epsilon = -1$ ($\zeta = \zeta_c = 1.25$). The characteristic distances (in units of $\hbar/m_e c$ are: R = 0.03 is the nuclear radius, $r_0 = 0.225$ is the radius of the well in the effective potential (2.15), and $\bar{r} = 0.31$ is the average radius of the given state.

here $\nu = 2\sqrt{\zeta^2 - \kappa^2}$, $K_{i\nu}$ is a Macdonald function with imaginary index (it is tabulated in [43]). The function $K_{i\nu}(x)$ is real for real values of ν and x and is even in the index ν; it can be defined by the integral

$$K_{i\nu}(x) = \int_0^\infty e^{-x \operatorname{ch} t} \cos \nu t \, dt, \qquad (2.23)$$

which converges rapidly and is convenient for numerical calculations. As $x \to \infty$, the function $K_{i\nu}(x)$ decreases exponentially:

$$K_{i\nu}(x) = \left(\frac{\pi}{2x}\right)^{1/2} e^{-x} \left(1 - \frac{\nu^2 + (1/4)}{2x} + \ldots\right), \qquad (2.24)$$

and as $x \to 0$ it has an infinite number of oscillations

$$K_{i\nu}(x) = \left(\frac{\pi}{\nu \operatorname{sh} \pi\nu}\right)^{1/2} \sin\left(\nu \ln \frac{2}{x} + \arg \Gamma(1 + i\nu)\right). \qquad (2.25)$$

The solution (2.22) for the potential (2.5) is suitable in the entire region $r > R$. In the internal region $r < R$ we can use the smallness of the nuclear radius R compared with the Compton wavelength of the electron.* Changing over in (2.9) to the dimensionless variable $x = r/R$ and discarding terms of order R, we obtain

$$\frac{dG}{dx} = -\frac{\kappa}{x} G + \zeta f(x) F, \quad \frac{dF}{dx} = -\zeta f(x) G + \frac{\kappa}{x} F; \qquad (2.26)$$

here f(x) are cutoff functions from (2.5). At an arbitrary form of f(x), these equations can be solved numerically.† To determine the level spectrum and ζ_c it suffices to obtain from (2.26) only one constant which we shall choose to be the logarithmic derivative of the function G(r) at the edge of the nucleus:

$$\xi = \left[\frac{r}{G}\frac{dG}{dr}\right]_{r=R}. \qquad (2.27)$$

The quantity ξ depends on ζ, κ, and on the form of the cutoff f(x) (but does not depend on the energy, as a result of the approximation $R \ll 1$). For a rectangular cutoff (i.e., $f(x) \equiv 1$), the solution can be obtained analytically

$$\xi = \xi_- = \zeta \operatorname{ctg} \zeta \quad \text{for} \quad \kappa = -1,$$
$$\xi = \xi_+ = \frac{\zeta^2}{1 - \zeta \operatorname{ctg} \zeta} - 1 \quad \text{for} \quad \kappa = +1.$$

The dependence of ξ on ζ for two cutoff models is shown in Fig. 4. Model I corresponds to f(x) = 1 (the entire charge is on the surface of the nucleus) and model II corresponds to a uniform distribution of the charge over the volume of the nucleus. With increasing ζ, the parameter ξ always decreases, with $\xi_+(\zeta) > \xi_-(\zeta)$.

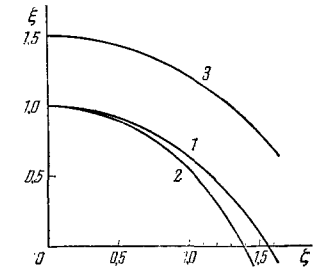

FIG. 4. Dependence of ξ on $\zeta = Z/137$. 1–1S level, cutoff model I; 2–1S level, model II; 3–$2P_{1/2}$ level, model II.

Matching of the solutions on the edge of the nucleus yields a transcendental equation for the critical charge $Z_c = 137\zeta_c$

$$z \frac{K'_{i\nu}(z)}{K_{i\nu}(z)} = 2\xi, \qquad (2.28)$$

where $\nu = 2\sqrt{\zeta_c^2 - 1}$, $z = \sqrt{8\zeta_c R}$ and $\xi = \xi(\zeta_c)$. We have put here $\kappa^2 = 1$, for in all other states, with the exception of $nS_{1/2}$ and $nP_{1/2}$, the values of ζ_c are too large and at $\zeta < 2$ we can use for them formula (2.1), which pertains to a point Coulomb field.

Let us investigate (2.28) qualitatively. The function $\psi_\nu(z) = zK'_{i\nu}(z)/K_{i\nu}(z)$ is shown in Fig. 5, together with a graphic solution of Eq. (2.28), which yields an infinite sequence of roots $z = z_n^{\pm}$ ($n = 1, 2, \ldots$). The ground level 1S corresponds (at given R) to a minimal ζ_c, which is equivalent to a maximum root Z_1^- (at fixed ζ). The remaining roots z_n^-, $n \geq 2$, correspond to those values of ζ, at which the level $nS_{1/2}$ reaches the limit of the lower continuum. The roots z_n^+ corresponding to ξ_+ yield ζ_c for the levels $nP_{1/2}$. It can be shown that $\xi_+ > \xi_-$ (see Fig. 4); therefore the roots are arranged in the sequence $z_1^- > z_2^+ > z_2^- > \ldots$. It follows therefore that at a specified nuclear radius R the values of Z_c for states with $j = 1/2$ lie in the following order: $1S_{1/2}$, $2P_{1/2}$, $3S_{1/2}$, $3P_{1/2}$, ...

These conclusions are fully confirmed by the numerical solution of Eq. (2.28), the results of which are shown in Fig. 6. Calculations of ζ_c were carried out for two cutoff models (models I and II, see above). The transition from model I to model II increases the maximum value of the potential V(0) at the same radius R by a factor 1.5, as a result of which ζ_c decreases. However, as seen from the figure, this decrease is small. If we extrapolate into the region $Z > 137$ the relation $R = r_0 A^{1/3}$, assuming (as for heavy nuclei) that $A = 2.5Z$ and $r_0 = 1.1F$, and use model II, then we obtain* $\zeta_c = 1.25$ and $Z_c = 1.25$ and $Z_c = 170$ (for the lower $1S_{1/2}$ level). For the closest next states $2P_{1/2}$ and $2S_{1/2}$, the values of Z_c are 185 and 220, respectively. These values of Z_c are quite stable against variations of the radius R and of the form of the cutoff function f(r/R), as follows from a comparison of curves I and II in Fig. 6.

We note that the "random" degeneracy of the states with respect to the sign of κ (see formula (2.1), which contains only $|\kappa|$), which is characteristic of the Coulomb field, is lifted when $\zeta > 1$. This is not surprising,

*Thus, for example, a radius $R = 1.2 \times 10^{-12}$ cm corresponds to R = 0.03 (in units of $\hbar/m_e c$).

†Actually, for a numerical calculation it is convenient to reduce (2.26) to a single first-order equation (but a nonlinear one) (see Eq. (7) in [10]).

*The values of Z_c are also given with good accuracy by the WKB method [44].

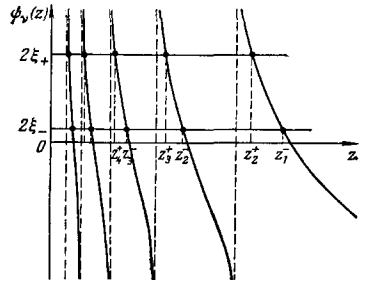

FIG. 5. Graphic solution of Eq. (2.28). The roots z_n^- correspond to the levels $nS_{1/2}$ ($\kappa = -1$) and the roots z_n^+ to the levels $nP_{1/2}$ ($\kappa = +1$).

since the potential V(r) in the region $r < R$ differs in principle from the "pure" Coulomb potential, and at $\zeta > 1$ the region of small r becomes significant (for states with $j = 1/2$).

2.5. Thus, the critical charge of the nucleus Z_c for any cutoff model can be calculated relatively simply. It is more difficult to obtain an idea of the character of the entire discrete spectrum at $Z > 137$, since the exact expressions for the wave functions at $\epsilon \neq \pm 1$ contain Whittaker functions and are quite cumbersome.* To simplify the situation, we assume that $R \to 0$; then a "large logarithm"

$$\Lambda = \ln \frac{1}{R} \gg 1 \qquad (2.29)$$

appears in the problem. Although numerically at R $\sim 10^{-12}$ cm the parameter Λ is still not very large ($\Lambda = 3.5$), to obtain a qualitative picture of the level motion such an approximation is sufficient.* We present first of all consideration favoring the fact that the small parameter in this problem is indeed Λ^{-1}.

1) Let first $\zeta < 1$. In the field of a point-like charge Ze the energy for the ground state is $\epsilon = \epsilon_1 = \sqrt{1-\zeta^2}$, and the wave functions are

$$G(r) = A\sqrt{1+\varepsilon}\, e^{-\zeta r} r^{\gamma}, \quad F(r) = -\sqrt{\frac{1-\varepsilon}{1+\varepsilon}}\, G(r) \qquad (2.30)$$

(the constant A is determined from the condition for the normalization of (2.6) and is equal to $A = 2\gamma\sqrt{\zeta^{2\gamma+1}/\Gamma(1+2\gamma)}$, $\gamma = \sqrt{1-\zeta^2}$).

Calculating the level shift due to the cutoff of the potential in (2.5) by perturbation theory, we obtain (at $R \ll 1$)

$$\Delta\varepsilon = \frac{\zeta^2 (2\zeta R)^{2\gamma}}{\gamma\Gamma(1+2\gamma)} \left\{1 - 2\gamma \int_0^1 f(x)\, x^{2\gamma}\, dx\right\}. \qquad (2.31)$$

The correction $\Delta\epsilon$ ceases to be small when $R^{2\gamma} = \exp(-2\gamma\Lambda)$ becomes of the order 1, i.e., at $(1-\zeta) \sim \Lambda^{-2}$.

2) Let us estimate the energy of the ground state at $\zeta = 1$ (such a value of ζ is critical for a point-like charge). In this case the functions G and F have a logarithmic singularity at zero: $G(r) \approx r^{\epsilon} = 1 + \epsilon \ln r$ as $r \to 0$, whence

$$\xi = \left[\frac{rG'}{G}\right]_{r=R} = \frac{\varepsilon}{1-\varepsilon\Lambda}, \qquad \varepsilon \approx (\Lambda + \xi^{-1})^{-1}. \qquad (2.32)$$

Since $\Lambda \gg 1$ and $\xi = 0(1)$, it follows that $\epsilon_1 \sim \Lambda^{-1}$ at $\zeta = 1$. The difference from the value $\epsilon_1 = 0$, which corresponds to a point-like charge, is quite appreciable. Thus, a numerical calculation[46] for R = 10.2F yielded $\epsilon_1 = 0.238$, which agrees well with the foregoing estimate.

3) At $\zeta > 1$ the wave functions for the problem with the point Coulomb potential have at zero a singularity characteristic of the "falling to the center":

$$G,\ F \underset{(r\to 0)}{\sim} \sin(g \ln r), \qquad (2.33)$$

where $g = \sqrt{\zeta^2 - 1}$.

Since the wave function of the ground state has no nodes, the $1S_{1/2}$ level can exist only when $g\Lambda < \pi$. The maximum possible values of g and ζ correspond to vanishing of this level in the lower continuum:

$$g_c = \frac{\pi}{\Lambda}, \quad \zeta_c = 1 + \frac{\pi^2}{2\Lambda^2}. \qquad (2.34)$$

It is clear from the foregoing that the parameter Λ determines both the width of that region about the point $\zeta = 1$ in which allowance for the finite dimensions of the nucleus is essential, as well as the dependence $\epsilon = \epsilon(\zeta)$ itself in this region.

Let us determine the type of the wave functions near $\zeta = 1$ (we confine ourselves for simplicity to the ground state). By analogy with (2.30) we put

$$\left.\begin{aligned} G(r) &= A\sqrt{1+\varepsilon}\, e^{-\rho/2}\rho^{\varepsilon}\left[1 - (\varepsilon^2 + g^2)\,\xi_1(\rho) + \ldots\right], \\ F(r) &= -A\sqrt{1-\varepsilon}\, e^{-\rho/2}\rho^{\varepsilon}\left[1 - (\varepsilon^2 + g^2)\,\xi_2(\rho) + \ldots\right] \end{aligned}\right\} \qquad (2.35)$$

($\rho = 2\lambda r$, $\lambda = \sqrt{1-\epsilon^2}$, $\epsilon, g \to 0$; we carry out the calculations accurate to terms quadratic in ϵ and g). Substitution of the expansions (2.35) in (2.9) yields equations

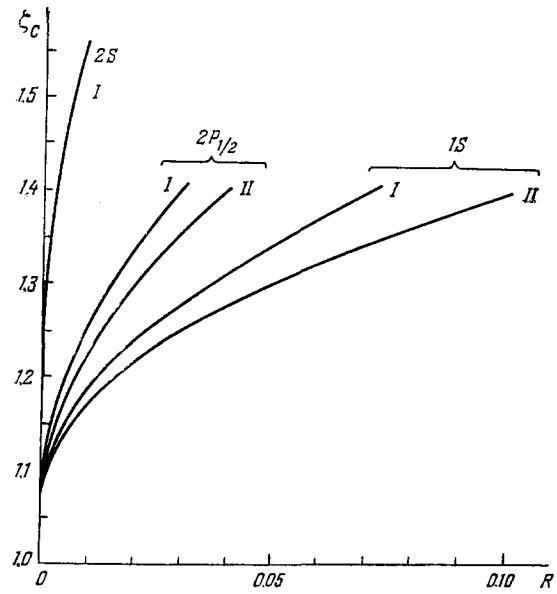

FIG. 6. Critical charge of the nucleus ($\zeta_c = Z_c/137$) for the first level with angular momentum $j = 1/2$. The numbers I and II at the curves correspond to the cutoff models I and II (see the text).

*See formulas (12)–(14) of [10]. An equation determining the level energy for model I is given in [10], and in the case of arbitrary cutoff in [12].

†A numerical calculation of the level motion was carried out in [45]. The values of Z_c obtained therein are in good agreement with those calculated from (2.28).

for the corrections ξ_1 and ξ_2, and their solution (which decreases at infinite) is of the form[12]

$$\xi_{1,2}(\rho) = \int_0^\infty dt e^{-\rho t}\left(\frac{\ln(1+t)}{t} \mp \frac{1}{2(1+t)}\right) \qquad (2.35')$$

(here $\xi_{1,2} \approx \ln^2 \rho/2$ as $\rho \to 0$).

In the region of r such that $r \ll 1$ and $g \ln(1/r) \ll 1$ we have

$$G \approx -F \approx 1 + \varepsilon \ln r - \frac{1}{2} g^2 \ln^2 r + \ldots \qquad (2.36)$$

On the other hand, when r ~ R we have G(r) = C sin (g ln r + β).

The phase β is determined from the condition of matching on the boundary of the nucleus:

$$\beta = g\Lambda + \arg \operatorname{tg}(g/\zeta) \approx g\Lambda \qquad (\text{for } \Lambda \gg 1).$$

In the region $R \ll r \ll 1$ we therefore obtain G(r) = C sin β(1 + g cot β ln r), which should coincide with (2.36). This yields

$$\varepsilon_1 = g \operatorname{ctg} \beta = g \operatorname{ctg} \Lambda g \qquad (2.37)$$

($g = \sqrt{\zeta^2 - 1}$). Unlike (1.1), this expression has no singularity at $\zeta = 1$. At $\zeta < 1$ it is necessary to replace g by $i\gamma$:

$$\varepsilon_1 = \gamma \operatorname{cth} \Lambda\gamma \qquad (\gamma = \sqrt{1-\zeta^2}). \qquad (2.37')$$

In the region $\zeta < 1$, the function coth $\Lambda\gamma$ tends rapidly to unity and already at $(1-\zeta)\Lambda^2 \gtrsim 1$ the energy ϵ_1 practically coincides with (1.1) and does not depend on the cutoff of V(r) inside the nucleus (Fig. 7). At $\zeta > 1$, the function (2.37) has a fictitious pole at $g = g_c = \pi/\Lambda$. In fact, of course, $\epsilon = -1$ at $\zeta = \zeta_c$, and not at $-\infty$. The point is that the approximate expansions (2.35) cease to valid when ϵ is not small. Taking (2.37) into account we obtain for the coefficient in front of the correction terms ξ_1 and ξ_2 in (2.35)

$$\varepsilon^2 + g^2 = \begin{cases} (\gamma/\operatorname{sh}\Lambda\gamma)^2 & \text{for } \zeta < 1, \\ (g/\sin \Lambda g)^2 & \text{for } \zeta > 1. \end{cases}$$

As $\zeta \to \zeta_c$, we have $(\epsilon^2 + g^2) \to \infty$, and therefore the expansion (2.35) becomes meaningless. The functions G and F are then no longer close to (2.30). For example, at $\zeta = 1$ for

$$\left.\begin{array}{l} G = -F = e^{-r}, \quad \text{if} \quad \varepsilon = 0, \\ G = cK_0(\sqrt{8r}),\ F = -c\{K_0(\sqrt{8r}) + \sqrt{2r}K_1(\sqrt{8r})\}, \quad \text{if} \quad \varepsilon = -1 \end{array}\right\} \qquad (2.38)$$

(here $c^2 = 12/5$; the functions G and F are normalized in accordance with (2.6)).

A more thorough investigation shows that near $\zeta = \zeta_c$ there is a narrow region $(\zeta_c - \zeta) \sim \Lambda^{-3}$, in which formula (2.37) for $\epsilon_1(\zeta)$ is not valid. We shall not present here the corresponding expression for the energy ϵ_1 of the level (it can be found in [12]). We shall only indicate that at $\zeta = \zeta_c$ the level $1S_{1/2}$ does not cling to the boundary $\epsilon = 1$, but enters into the lower continuum, having a finite derivative $\partial\epsilon/\partial\zeta$:

$$\varepsilon_1(\zeta) = -1 + \frac{3\Lambda^3}{5\pi^2}(\zeta_c - \zeta). \qquad (2.39)$$

A similar behavior is exhibited also by all the remaining levels of the discrete spectrum. Thus, for the excited states $nS_{1/2}$ and $nP_{1/2}$ we have

$$\varepsilon_n(\zeta) = \frac{n-1}{N} + \frac{g \operatorname{ctg} \Lambda g}{N^3}, \quad N = \sqrt{n^2 - 2n + 2}. \qquad (2.40)$$

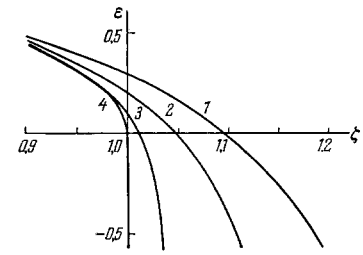

FIG. 7. Energy of ground state 1S near Z = 137. Curves 1–4 correspond to Λ = 3.5, 5, 10 and ∞ (cutoff radius R = 12, 2.6, 0.18 F and R = 0, respectively).

Although at $n \gg 1$ these states lie already in the nonrelativistic region $\epsilon \approx +1$, they are also sensitive to the cutoff of the Coulomb potential at short distances. Since $\epsilon_{n+1} - \epsilon_n \sim n^{-3}$, the shift of the level ϵ_n as a result of the finite dimensions of the nucleus is much smaller than the distance between the neighboring levels, so long as $g\Lambda < \pi$. On the other hand, when $g \to g_c = \pi/\Lambda$, the energies ϵ_n vary rapidly with increasing ζ. As $\zeta = \zeta_c$ the levels $1S_{1/2}$ and $2P_{1/2}$ go over into the lower continuum,* and for the remaining states with $j = \frac{1}{2}$ the picture is the same as if the principal quantum number n were to be decreased by unity (see Fig. 1b). With further increase of ζ, these phenomena repeat. The critical values $\zeta_c^{(n)}$ for the levels $nS_{1/2}$ and $nP_{1/2}$ are equal to, accurate to terms $\sim\Lambda^{-3}$,

$$\zeta_c^{(n)} = 1 + \frac{n^2\pi^2}{2\Lambda^2} \quad \left(g_c^{(n)} = \frac{n\pi}{\Lambda}\right), \qquad (2.41)$$

i.e., they increase rapidly with increasing n.

2.6. Let us dwell also on the question of the dimensions of the bound state. We take the lower level 1S. So long as $\zeta < 1$, we can use the wave functions (2.30) for a point Coulomb potential, which yields

$$\bar{r} = \frac{1 + 2\sqrt{1-\zeta^2}}{2\zeta} \qquad (0 < \zeta < 1). \qquad (2.42)$$

Calculation of $\bar{r}$ for $\zeta > 1$ becomes much more complicated. We therefore present only the final result.[10] At $\epsilon = -1$ ($Z = Z_c$) we have for $\kappa = -1$

$$\bar{r} = \frac{(4\zeta_c^2 - 3)(1 + 0{,}3\zeta_c^2)}{2\zeta_c(3 + 2\zeta_c^2)}. \qquad (2.43)$$

In accordance with the statement made above (see formulas (2.17) and (2.19), the average radius $\bar{r}$ at $\epsilon = -1$ remains finite (thus, at $\zeta_c = 1.25$ we get $\bar{r} = 0.3$), i.e., the bound state is not delocalized as $Z \to Z_c$. This occurs in spite of the fact that the exponential $\exp(-\lambda r)$, which leads to the damping of $\psi(r)$ as $r \to \infty$ for bound

*In the asymptotic formulas (2.37) and (2.40) we have left out terms of the order of unity compared with Λ. In this approximation, the energy ϵ_n does not depend on the form of the cutoff of the potential inside the nucleus (all that matters is the cutoff radius R), and the values of $\zeta_c^{(n)}$ for the levels $nS_{1/2}$ and $nP_{1/2}$ coincide (in fact, $H\zeta_c \sim \Lambda^{-3}$ for these states).

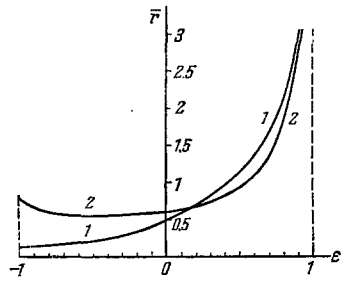

FIG. 8

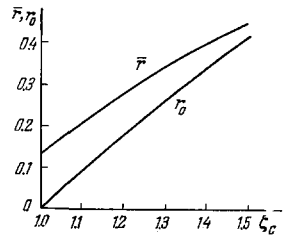

FIG. 9

FIG. 8. Average radius $\bar{r}$ for the ground state in the Coulomb field (2.5) in the case $\Lambda \gg 1$. Curves 1 and 2 correspond to particles with spin s = 1/2 and 0. $\bar{r}$ is measured in units of $\hbar/mc$.

FIG. 9. Average radius $\bar{r}$ of the ground state 1S at $\epsilon = -1$, and well radius r_0 in the effective potential U(r).

states in ordinary atoms, is not effective in this case ($\lambda = \sqrt{1-\epsilon^2} = 0$ at $\epsilon = -1$). The reason for the localizability of the wave functions at $\zeta = \zeta_c$ and $\epsilon = -1$ is the Coulomb barrier in the effective potential U(r). Figure 8, which is taken from [10], shows how the average radius of the ground state 1S varies when the level deepens from $\epsilon = 1$ to $\epsilon = -1$. A comparison of $\bar{r}$ with the well radius $r_0 = (\zeta^2 - 1)/2\zeta$ in U(r) is shown in Fig. 9, from which it is seen that at $\epsilon = -1$ the electron spends a considerable fraction of the time under the barrier, i.e., in the classically inaccessible region ($r > r_0$).

The analytic expressions for $\bar{r}$ in the intermediate region $1 < \zeta < \zeta_c$ are very cumbersome,[10] but do not lead to anything unexpected. As ζ increases from 1 to ζ_c, the bound state of the electron continues to contract (see Fig. 8), and the point $\zeta = \zeta_c$ itself is not a singularity for the function $r = r(\zeta)$.

The other characteristics of the level, for example the magnetic moment, behave in similar fashion.[47]

3. PERTURBATION OF CONTINUOUS SPECTRUM BY A NEARBY LEVEL

To understand the situation at $Z > Z_c$, it is necessary to determine first what happens to the wave functions of the continuous spectrum when a discrete level approaches this spectrum. This question, which is of interest in itself, will be analyzed first using nonrelativistic quantum mechanics as an example.

3.1. If the system has a level (real or virtual) with low energy, then the wave functions $\chi_k(r)$ of the continuous spectrum should experience a certain perturbation as $k \to 0$ (k is the momentum, and the point k = 0 corresponds to the boundary of the continuous spectrum). This question was considered by Zel'dovich and Rabinovich[20] as applied to a degenerate Fermi gas,* and was investigated recently in detail in [23,24].

The result of [20] reduces intuitively to the fact that the entire aggregate of the levels below a given energy ϵ_f (i.e., the aggregate of electrons filling the levels below the Fermi boundary) constitutes an entity, perturbation of which occurs near the boundary $\epsilon = \epsilon_f$. The distribution of the total electron density in coordinate space remains unchanged when variation of the potential relief (of the function V(r)) gives rise to the appearance or to the vanishing of levels of the discrete spectrum. But this is possible only when the appearance or vanishing of the discrete level is accompanied by a realignment of the wave functions of the continuous spectrum, which cancels the contribution of this level. We now formulate this result more accurately.

First, it is easy to obtain an integral characteristic of the perturbation of the functions $\chi_k(r)$. To this end, following [20], we use the completeness theorem. Let v be a quantity determining the depth of the potential,* and let the first bound level arise at $v = v_c$. Writing down the completeness relation for $v_1 < v_c$ and $v_2 > v_c$

$$\int_0^\infty dk \chi_k^*(r; v_1)\chi_k(r'; v_1) = \delta(r-r'),$$

$$\chi_0(r)\chi_0(r') + \int_0^\infty dk \chi_k^*(r; v_2)\chi_k(r'; v_2) = \delta(r-r'),$$

subtracting one equation from the other, and then putting $r' = r$, we obtain

$$\chi_0^2(r; v_2) = \int_0^\infty dk \{|\chi_k(r; v_1)|^2 - |\chi_k(r; v_2)|^2\}; \qquad (3.1)$$

here $\chi_k(r)$ are the wave functions with orbital angular momentum l normalized to $\delta(k - k')$:

$$\chi_k(r) \underset{(r\to\infty)}{\approx} \sqrt{\frac{2}{\pi}} \sin\left(kr - \frac{l\pi}{2} + \delta\right), \qquad (3.2)$$

$\delta = \delta_l(k)$ is the scattering phase. The wave function of the level $\chi_0(r)$ corresponds to the usual normalization of the discrete spectrum (at $v > v_c$)

$$\int_0^\infty \chi_0^2(r)\, dr = 1. \qquad (3.3)$$

Let us see now what happens to (3.1) as $v_2 \to v_c$ and when r is fixed.

It is necessary to distinguish here between two cases, depending on the behavior of the potential V(r) as $r \to \infty$. If $l = 0$ and $V(r) \leq 0$ at sufficiently large r (the case of attraction), or else if the sign of V(r) is arbitrary, but $\lim_{r\to\infty} r^2 V(r) = 0$, then delocalization of the wave function of the bound state takes place: $\chi_0(r) \sim \sqrt{2\lambda}\, e^{-\lambda r}$, and $\lambda \to 0$ as $v_2 \to v_c$. In this case the bound state "swells up" and the wave function $\chi_0(r)$ at the instant of vanishing of the level can no longer be normalized in accordance with (3.3). As the normalization condition we can choose here

$$\lim_{r\to\infty} \chi_0(r) = 1. \qquad (3.4)$$

On the other hand, if V(r) has at infinity a barrier of the Coulomb type,

$$V(r) \approx \zeta r^{-n} \qquad (\zeta > 0,\ 1 \leq n < 2) \qquad (3.5)$$

(and also in the case $l \geq 1$, when there is a centrifugal barrier $l(l+1)/2r^2$), then the function $\chi_0(r) \equiv \chi_c(r)$ decreases rapidly as $r \to \infty$ at the instant of occurrence of the level ($v = v_c$), and therefore the normalization

*See also [22], p. 205. A mathematical justification for the results obtained in [20] is given in [21].

*See, for example, formula (2.5), where the parameter v coincides with ζ. For what follows, however, it is not at all necessary that v enter in V(r) only as a common factor.

(3.3) remains in force for it. For example, in the case of greatest physical interest, that of a Coulomb "tail" ($V(r) \approx \zeta/r$ ($\zeta > 0$), we have

$$\chi_c(r) \approx A\,(r/2\zeta)^{1/4}\, e^{-\sqrt{8\zeta r}}, \tag{3.6}$$

and if $\lim_{r\to\infty} r^2 V(r) = 0$ but $l \geq 1$, then $\chi_l^{(n)}(r) \sim r^{-l}$.

There exists here a limit $\lim_{v\to v_c} \chi_0(r; v) = \chi_c(r)$, and at the instant when the level appears the function $\chi_c(r)$ is square-integrable.

Different behaviors of the wave function $\chi_c(r)$ as $r \to \infty$ corresponds also as a different course of the energy of the level ϵ as a function of the parameter v that determines the depth of the well. It is obvious that the derivative $\partial\epsilon/\partial v$ is proportional to the probability that the particle will stay inside the well, i.e., to the quantity $\int_0^R \chi_0^2(r)\,dr$ (for details see [22], p. 20). In the deuteron case, owing to delocalization, we have $\chi_0^2(r) \sim \lambda = \sqrt{-2\epsilon}$, so that $\partial\epsilon/\partial v \sim \sqrt{-\epsilon}$ and therefore $\epsilon = -c(v - v_c)^2$, where $c > 0$ is a certain constant. The curve $\epsilon = \epsilon(v)$ touches the abscissa axis at $v = v_c$, and the level deepens in proportion to the square of $v - v_c$.

In the case of a potential with a Coulomb barrier, the derivative $\partial\epsilon/\partial v$ is finite at $v = v_c$ and therefore the level deepens linearly: $\epsilon = -c'(v - v_c)$. When $v < v_c$, the $\epsilon = \epsilon(v)$ curve goes off at a finite slope to the continuous spectrum, where it represents the resonance energy. At small $(v_c - v)$ we have

$$\mathrm{Re}\,\varepsilon = c'(v_c - v),\ \mathrm{Im}\,\varepsilon = \begin{cases} \text{const}\cdot\exp\left(-\dfrac{a}{\sqrt{v_c - v}}\right) & \text{for } v < v_c, \\ 0 \text{ for } v > v_c, \end{cases} \tag{3.7}$$

where $b = 2\pi\zeta/\sqrt{2c'}$.

From relation (3.1), in which v_1 and v_2 are close to v_c, we see that at $v < v_c$ one particle already "sits," as it were, in the continuous spectrum, and the density of the perturbation of the functions $\chi_k(r)$ has the same spatial localization as the function $\chi_c(r)$. The connection between $\chi_k(r)$ and $\chi_c(r)$ can be written in greater detail in the form

$$\chi_k(r) \approx \sqrt{\Delta(k)}\,\chi_c(r). \tag{3.8}$$

As $k \to 0$, this relation is valid in the wide region $0 < r \ll k^{-1}$, including everywhere under the barrier. The factor $\Delta(k)$ changes strongly in the resonant energy region. Let us consider first potentials with finite barrier penetrability at $k = 0$, when delocalization of the bound state takes place and the normalization condition for $\chi_c(r)$ must be taken in the form (3.4). It can then be shown[23] that ($l = 0$)

$$\Delta(k) = \frac{8\varkappa^2 k^2}{\pi\left[(k^2 - k_0^2)^2 + 4\varkappa^2 k^2\right]}, \tag{3.9}$$

where we have introduced the parameters k_0^2 and $\varkappa$:

$$k_0^2 = 2/r_0 a, \quad \varkappa = -1/r_0 \tag{3.10}$$

(a is the scattering length and r_0 the effective radius).

In the region of interest to us near resonance we have $|a| \gg R$, and $a > 0$ for a real level and $a < 0$ for a virtual one (R is the effective radius of the potential). The quantity r_0 can be expressed directly in terms of the wave function $\chi_c(r)$ (see [39,48]): $r_0 = 2\int_0^\infty dr\,[1 - \chi_c^2(r)]$ (this integral converges by virtue of the boundary condition (3.4)). For an attraction potential $V(r) \leq 0$ we have $\chi_c(r) \leq 1$ and therefore $r_0 \sim R > 0$. On the other hand, if there is a barrier in $V(r)$, then r_0 can reverse sign (for this reason, the very designation "effective radius" becomes somewhat arbitrary here). For a broad barrier $r_0 \approx -R/\xi$, where ξ is the penetrability of the barrier ($\xi \ll 1$). Then $\varkappa > 0$ and is exponentially small ($\varkappa \sim \xi$), and k_0^2 can have any sign, with $k_0 = 0$ at the instant when the real level appears (the scattering length $a \to \infty$).

The parameters k_0^2 and $\varkappa$ determine the positions of the S-matrix poles that are close to zero. If $k_0^2 < \varkappa^2$, then the poles lie on the imaginary axis: $k = i\lambda$,

$$\lambda_1 = \sqrt{\varkappa^2 - k_0^2} - \varkappa, \quad \lambda_2 = -(\sqrt{\varkappa^2 - k_0^2} + \varkappa). \tag{3.11}$$

When $k_0^2 < 0$, the first pole corresponds to a real level, and the second to a virtual one. At $k_0^2 = 0$, the real level vanishes, going over to the lower half-plane $\mathrm{Im}\,k < 0$. In the interval $0 < k_0^2 < \varkappa^2$ the poles are virtual; they collide at $k_0^2 = \varkappa^2$ and go off to the complex plane:

$$k_{1,2} = \pm\sqrt{k_0^2 - \varkappa^2} - i\varkappa. \tag{3.12}$$

Finally, at $k_0^2 \gg \varkappa^2$ these poles correspond to the Breit-Wigner resonance $E = \epsilon_0 - (i\gamma/2)$, where $\epsilon_0 = k_0^2/2$, and $\gamma = 2\varkappa k_0$ ($\epsilon_0 \gg \gamma$). Formula (3.9) then assumes a form[49] typical of the quasistationary level (Lorentzian line shape):

$$\Delta(\varepsilon) = \frac{\Delta(k)}{k} = \frac{\gamma}{2\pi\left[(\varepsilon - \varepsilon_0)^2 + \gamma^2/4\right]}. \tag{3.13}$$

Expression (3.9) is more general than (3.13), and covers all locations of the poles on the complex k plane.

From the point of view of analyticity, the pole motion described above is quite natural.[50] In the case when there is no barrier, however, the collision of the poles occurs far from zero (at $|k| \sim R^{-1}$), and can therefore not be described within the framework of the low-energy expansion for the S matrix. This is the situation, for example, in the case of the deuteron:[51,52] $|a| \gg R$, $r_0 \sim R > 0$. An important feature of a potential with a broad barrier is the fact that at $\lambda_1 \to 0$ the virtual level $k_2 = i\lambda_2$ is also exponentially close to zero, by virtue of which the two parameters k_0^2 and $\varkappa^2$ suffice to describe all the phenomena connected with the collision of the poles.

Formula (3.8) shows the appearance of the perturbation of the wave functions $\chi_k(r)$ when a level goes off to the continuous spectrum. At an arbitrarily chosen energy, the $\chi_k(r)$ attenuate exponentially in the interior of the barrier, so that $\chi_k(R)/\chi_k(L) \sim \xi^{1/2} \ll 1$.* In the narrow region $|\epsilon - \epsilon_0| \sim \gamma$, however, the function $\chi_k(r)$ has a form similar to that of $\chi_0(r)$, i.e., a strong increase takes place in the probability of the particle staying inside the well ($r < R$). To describe this perturbation of the functions $\chi_k(r)$, we introduce the concept of the effective particle number N, to which the entire continuous spectrum is equivalent (in a certain sense). To this end we change over from $\chi_0(r)$ to the approximate wave function $\tilde{\chi}_0(r)$, for which the normalization integral (3.3)

*Here R is the radius of the internal well, L is the end of the barrier (the turning point), and $\xi = \exp\{-2\int_L^A |p(r)|\,dr\} \ll 1$.

converges. The transition is carried out as follows:[23]

$$\tilde{\chi}_0(r) = \sqrt{2\varkappa}\{\chi_0^2(r) - 1\}^{1/2} \qquad (3.14)$$

(at r not too close to the edge of the barrier L we have $\chi_0(r) \gg 1$ and therefore $\chi_0(r)$ and $\tilde{\chi}_0(r)$ are proportional to each other). The function $\tilde{\chi}_0(r)$ describes a particle state localized inside the barrier. Realizing (3.8) at $r < L$ in the form $\chi_k(r) = \sqrt{\nu(k)}\,\tilde{\chi}_0(r)$, we obtain

$$N = \int_0^\infty \nu(k)\,dk = \begin{cases} \dfrac{\varkappa}{\varkappa+\lambda_1} = \dfrac{\varkappa}{\sqrt{\varkappa^2 - k_0^2}} & \text{for } k_0^2 < 0, \\ 1 & \text{for } k_0^2 > 0. \end{cases} \qquad (3.15)$$

At $\lambda_1 \gg \kappa$ we have $N \ll 1$; the number N becomes of the order of unity when the level energy approaches zero. As soon as the level enters the continuous spectrum ($k_0^2 > 0$) we have N = 1.

Thus, the influence of the real level on the continuous-spectrum function $\chi_k(r)$ exists in a very narrow energy region ($|\epsilon_1| \sim \kappa^2$) and vanishes rapidly when this level becomes deeper. On the other hand, if the level goes off to the continuous spectrum, then the functions $\chi_k(r)$ exhibit rises at small r near the resonant energy $\epsilon = \epsilon_0$. This increase of $|\chi_k(r)|^2$ is equivalent to one particle situated in the state $\tilde{\chi}_0(r)$.

In the limit of a very broad barrier (and all the more for a potential with a Coulomb barrier) N is transformed into a step-like function: $N = \theta(k_0^2)$. The function $\tilde{\chi}_0(r)$ coincides with $\chi_c(r)$, while the factor $\Delta(k)$ vanishes when $k_0^2 < 0$ and has the Lorentz form (3.13) at $k_0^2 > 0$. So long as the level is real ($k_0^2 < 0$), its influence on the functions $\chi_k(r)$ is in this case practically nonexistent.

3.2. We proceed to the relativistic case. It was shown in Sec. 2 that a barrier is produced in the effective potential U(r) of the Dirac equation at $\epsilon \approx -1$, as a result of which the wave function remains normalizable at $\epsilon = -1$ (there is no delocalization). Owing to the spin term $U_2(r)$ of (2.13), this barrier has a zero penetrability at k = 0, even if the initial potential V(r) does not contain a Coulomb repulsion "tail." Thus, if $V(r) \approx -\alpha n^{-n}$ ($n > 2$) as $r \to \infty$, then it follows from (2.14) that

$$U(r) \underset{(r\to\infty)}{\approx} \frac{1}{2r^2}\left[\left(\varkappa + \frac{1-n}{2}\right)^2 - \frac{1}{4}\right] \qquad (3.16)$$

i.e., a barrier of the centrifugal type appears in U(r). If $V(r) \approx -\alpha e^{-\mu r}$, then the wave function attenuates exponentially. Thus, the function G(r) always remains square-integrable at $\epsilon = -1$. Therefore at $\zeta < \zeta_c$ the distortion of the wave functions of the lower continuum by a discrete level approaching the continuum is negligibly small, and at $\zeta > \zeta_c$ the functions $G_k(r)$ and $F_k(r)$ increase rapidly in the subbarrier region r (its enhancement takes place, of course, only in a narrow energy band near the resonance $\epsilon = \epsilon_0$; see Fig. 10). Relations of this kind have turned out to be quite useful for the calculation of the probability of two-proton decay,[49] for the solution of the problem of two interacting particles in a potential well, etc.

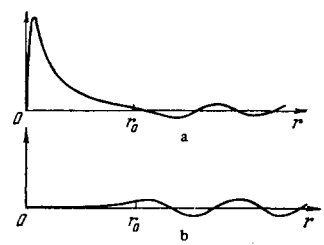

FIG. 10. Qualitative form of the lower continuum at $Z > Z_c$. a) In the energy and $|\epsilon - \epsilon_0| \sim \gamma$; b) at $|\epsilon - \epsilon_0| \gg \gamma$. Here $r_0 = 2\zeta|\epsilon|/(\epsilon^2 - 1)$ is the turning point.

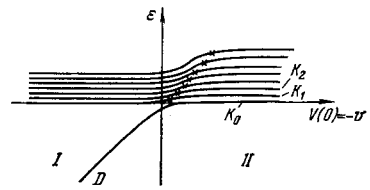

FIG. 11. Spectrum of levels in a box (k_0, k_1, ... are the continuum levels).

At $r \ll k^{-1}$ we can write

$$G_k(r) = \sqrt{\Delta(k)}\,G_c(r), \quad F_k(r) = \sqrt{\Delta(k)}\,F_c(r), \qquad (3.17)$$

where G_c and F_c are the wave functions for $\epsilon = -1$, normalized in accordance with (2.6), and the factor $\Delta(k)$ is given by (3.13).

The factorization of $\chi_k(r)$ in the form (3.8) is very convenient in the calculation of the matrix elements, for example

$$\left.\begin{aligned} &(\chi_k, V\chi_0) = \sqrt{\Delta(k)}\,V_{00}, \\ &\int dk\,dk' f(k,k')\,|(\chi_k, V\chi_0)|^2 = |V_{00}|^2 \int dk\,dk' f(k,k')\,\Delta(k)\,\Delta(k'). \end{aligned}\right\} \qquad (3.18)$$

Finally, we note a paradox that appears when a system is placed in a "large box" of radius R, when the spectrum changes from continuous to discrete.* Since the wave functions $\chi_n(r)$ are real, the number of the level n now coincides with the number of nodes of the radial function $\chi_n(r)$ (we confine ourselves for simplicity to an S-wave, $l = 0$). Let us see what happens if a potential well V(r) with a barrier is placed in the center of the box, and the depth v of the well varies ($v = -V(0) > 0$). We begin with the situation of a deep well ($v > v_c$; see region I in Fig. 11). Here we have a "truly discrete" level D which has no nodes; the "continuum" begins with a wave function with one node, etc.† We decrease the depth of the well v. At $v = v_c$, a value ϵ_1 is reached and the "truly discrete" level vanishes. At $v < v_c$ the spectrum consists only of closely lying levels with $\epsilon > 0$ ($\Delta\epsilon = \epsilon_{n+1} - \epsilon_n \sim R^{-2}$). Which level of the continuum in region II is a continuation ("successor") of the lower level D in the left side of Fig. 11? The formal answer is that this "successor" is the lower level k_0 on the right—it is just as much a "zero" level, and has likewise no nodes, as is the level D on the left.

However, singularities of the resonant type are ob-

*It is quite natural by itself to desire to reduce the less intuitive concept of the continuum (including normalization to a δ function, the concept of measure in the continuous spectrum, and other complications) to the simple case of a discrete spectrum, where the levels can be counted on the fingers—first, second, etc.

†For a system in a box, the terms "truly discrete level" and "continuum" are used, so to speak, in the Pickwickian sense [64], indicating the levels that replace them when $R \to \infty$.

served for scattering not by this level, but by the levels marked by the crosses, which precisely form in the region $\epsilon > 0$ the function $\epsilon = \epsilon(v)$ which contains the curve D for the "truly discrete" level. It is precisely these levels, which slide when v is varied, which are the true continuations of D.

An analysis of a hypothetical experiment with a particle bound in a state D and of its behavior when the depth of the well varies with time, $v = v(t)$, shows that the particle is emitted from one of the levels marked by a cross in Fig. 11.* As applied to the Coulomb problem with $Z > Z_c$, it can be stated that the wave functions $G_\epsilon(r)$ and $F_\epsilon(r)$, at $Z > Z_c$ and at ϵ close to -1 (it is immaterial whether $\epsilon < -1$ or $\epsilon > -1$), are not at all similar (in the region $r \sim 1$) to the wave functions $G_c(r)$ and $F_c(r)$ of the 1S level at the critical point $Z = Z_c$. On the other hand, in the narrow energy band of the lower continuum $|\epsilon - \epsilon_0| \lesssim \gamma$, the relation (3.17) is satisfied, from which it is clear that the analytic continuation of the $1S_{1/2}$ level in the transcritical region should be taken to be precisely the set of continuous-spectrum states with energy ϵ near the Breit-Wigner pole $E = \epsilon_0 - (i\gamma/2)$ (at least so long as $|1 + \epsilon_0| \ll 1$ and the width γ is small).

What is the cause of the temptation to erroneously regard just the lower level K_0 as a continuation of D? Let us recall the universally known picture of the intersection of two discrete levels in the theory of molecular spectra (Fig. 12a). Everyone knows that an arbitrarily small interaction moves the levels apart and causes the intersection to vanish (Fig. 12b). In the case of a small interaction and a finite rate of change of the parameter, however, this divergence remains purely formal, the system readily jumps through the gap, and moves in the manner shown by the arrows.

In our example, the introduction of the box turned out to be that small interaction which caused the vanishing of the intersection of the level with the continuum and gave rise to the error.

Is it worthwhile to examine in such detail the possible error? We cite in this connection the words of Nils Bohr: "A specialist is not one who worked much in a given field. A specialist is one who knows certain rough errors in a given field and is able to avoid them" (cited from Heisenberg's book[57]).

4. POSITRON PRODUCTION AND POLARIZATION OF VACUUM AT $Z > Z_c$

Let us proceed to discuss the phenomena occurring directly at the "critical point" $Z = Z_c$.

4.1. We expand the field operator $\psi(x)$ in terms of the exact solutions† of the Dirac equation in the Coulomb field of the nucleus Z:

$$\psi(x) = \sum_{(+)} a_n \psi_n(x) + \sum_{(-)} b_n^+ \bar{\psi}_n(x). \tag{4.1}$$

*It is curious that analogous situations occur also in the seemingly remote region of atomic and ionic collisions; the role of the parameter v(t) is played there by the distance R(t) between the colliding nuclei [55,56]. We confine ourselves here to an indication of the similarity between the kinetics of the process of detachment of the electron at finite velocity of the atoms to the kinetics of the production of positrons when two subcritical nuclei collide.

†The functions $\psi_n(x)$ include a time dependence, i.e., $\psi_n(x) = \psi_n(r) \exp(-i\epsilon_n t)$.

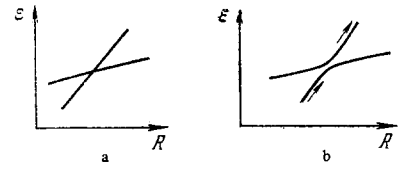

FIG. 12

Here (+) denotes the sum over the electronic states (i.e., the sum over the states of the discrete spectrum $-1 < \epsilon_n < 1$ and the integral over the upper continuum $\epsilon > 1$), and (−) denotes the sum over the positron states (lower continuum, $\epsilon < -1$). All the levels with energy $-1 < \epsilon_n < 1$ are classified as electronic states, for when Z is adiabatically decreased they return to the upper continuum. It is important that when $Z < Z_c$ there is no entanglement of the electronic and positronic states: as follows from (2.7), any level of the discrete spectrum appears from the upper continuum and drops monotonically with increasing Z. For particles obeying the Dirac equation, there are no levels that go from the lower continuum (i.e., there are no bound states for the antiparticles at a given sign of the potential $V(r) < 0$, in spite of the effective attraction $U_{eff} \sim -V^2/2$ at small distances, which takes place for both particles and antiparticles). We note immediately that this property of the solutions is typical precisely of the Dirac equation (in other relativistic equations the levels come from both the upper and the lower continuum).

Let us consider the Heisenberg current operator

$$j_\mu(x) = -\frac{e}{2}[\bar{\psi}(x), \gamma_\mu \psi(x)], \tag{4.2}$$

where $-e$ is the charge of the electron ($e > 0$). The mean value of $j_0(x)$ in an arbitrary state φ determines the charge density

$$\rho(\mathbf{r}) = \langle \varphi | j_0(x) | \varphi \rangle = -e \sum_{(+)} N_+ |\psi(\mathbf{r})|^2 + e \sum_{(-)} N_- |\psi(\mathbf{r})|^2 + \frac{e}{2}\left\{ \sum_{(+)} |\psi(\mathbf{r})|^2 - \sum_{(-)} |\psi(\mathbf{r})|^2 \right\} \tag{4.3}$$

where $N_+ = \langle a_n^+ a_n \rangle$ and $N_- = \langle b_n^+ b_n \rangle$ are the occupation numbers (the spatial part of the current j(x) gives zero when averaged over the stationary state φ). The last term in (4.3) is obviously the charge density of the vacuum*

$$\rho_{vac}(\mathbf{r}) = \frac{e}{2}\left\{ \sum_{(+)} |\psi_n(\mathbf{r})|^2 - \sum_{(-)} |\psi_n(\mathbf{r})|^2 \right\}. \tag{4.4}$$

We call here the state with $N_+ = N_- = 0$ the vacuum state (in the language of the initial Dirac theory this corresponds to a completely filled lower continuum). It is convenient to retain this definition, which is obvi-

*Strictly speaking, it would be necessary to add to (4.4) also the term term [58]

$$-\frac{e}{2}\delta(\mathbf{r}) \int d^3r' \left\{ \sum_{(+)} |\psi_n(r')|^2 - \sum_{(-)} |\psi_n(r')|^2 \right\},$$

which corresponds to regularization of the polarization operator $\Pi_R(k^2) = \Pi(k^2) - \Pi(0) - \Pi'(0)k^2$. This term makes no contribution when $r > 0$, and we shall omit it.

ous when $Z < Z_c$, also in the region of supercritical $Z > Z_c$. For a three-particle ($Z = 0$), the density $|\psi_\epsilon(r)|^2$ does not depend on the sign of ϵ, and therefore $\rho_{vac}(r) \equiv 0$.

In the field of the nucleus Z, the wave functions cease to be symmetrical with respect to the sign of ϵ. The resultant distortion $|\psi_\epsilon(r)|^2 - |\psi_{-\epsilon}(r)|^2$ determines the charge density induced in the vacuum (i.e., the polarization of the vacuum). So long as $Z < Z_c$, the total charge of the vacuum remains equal to zero

$$Q_{vac} = \int \rho_{vac}(r)\, d^3r \equiv 0. \tag{4.5}$$

This fact is immediately obvious if the system is placed in a large box of dimension L ($L \to \infty$). Then the spectrum becomes discrete ($\Delta\epsilon \sim L^{-2}$ when $|\epsilon| > 1$), and can trace the motion of each level. Since the wave functions $\psi_n(r)$ are normalized to unity over the volume of the box L^3 and the total number of levels remains unchanged with increasing Z, in the expression for Q_{vac} at $Z < Z_c$ a mutual cancellation of the contributions from the electronic and positronic states takes place (just as in the case of $Z = 0$).

If we substitute in (4.4) the exact Coulomb functions and carry out the summation, we can calculate in this way the polarization of the vacuum in a strong Coulomb field. Unfortunately, these calculations (if the parameter $\zeta = Z\alpha$ is not assumed small) turn out to be exceedingly cumbersome[15] and are not sufficiently complete to provide an easy-to-understand answer. It can be shown, however,* that when $\zeta \ll 1$ formula (4.4) leads to the well known Uehling potential:[59,60]

$$\varphi(r) = \varphi_0 + \delta\varphi = Ze\left\{\frac{1}{r} + \frac{2\alpha}{3\pi}\int\limits_{2m_e}^{\infty} d\mu\,\sigma(\mu)\,\frac{e^{-\mu r}}{r}\right\}, \tag{4.6}$$

where

$$\sigma(\mu) = \frac{\sqrt{\mu^2 - 4m_e^2}}{\mu^2}\left(1 + \frac{2m_e^2}{\mu^2}\right).$$

Let us analyze the polarization of vacuum in this approximation ($\zeta \ll 1$). It follows from (4.6) that

$$\varphi(r) = \frac{Ze}{r}\cdot\begin{cases} 1 + \dfrac{\alpha}{4\sqrt{\pi r^3}}\, e^{-2r} & \text{for } r \gg 1, \\ 1 + \dfrac{2\alpha}{3\pi}\ln\dfrac{1}{r} & \text{for } r \ll 1. \end{cases} \tag{4.7}$$

When $r \gg \hbar/m_e c = 1$, the polarization of vacuum gives exponentially small increments to the Coulomb potential $\varphi_0(r) = Ze/r$, and when $r \ll 1$ the deviation from Coulomb's law changes with distance logarithmically.

Taking into account the identity

$$(\Delta - \mu^2)\frac{e^{-\mu r}}{r} = -4\pi\delta(r),$$

we obtain the charge density corresponding to (4.6)

$$\rho(r) = -\frac{1}{4\pi}\Delta\varphi = Ze\left\{\delta(r) + \frac{2\alpha}{3\pi}\int\limits_{2m_e}^{\infty} d\mu\,\sigma(\mu)\left[\delta(r) - \frac{\mu^2 e^{-\mu r}}{4\pi r}\right]\right\}. \tag{4.8}$$

The charge distribution has the following form: a point-like positive charge $(1 + \gamma)Ze$ at the center $r = 0$, and a cloud of negative charges (adding up to $-\gamma Ze$), smeared out over a distance $r \sim 1$ from the nucleus. The total charge of the system is Ze, as follows formally from the identity

$$\int d^3r\left[\delta(r) - \frac{\mu^2 e^{-\mu r}}{4\pi r}\right] = 1 - 1 = 0$$

(γ is actually infinite, since it is given by the logarithmically-divergent integral $\gamma = \int\sigma(\mu)\,d\mu$). In the region $1/\alpha \gg \ln(1/r) \gg 1$, the density of the induced charges is equal to

$$\rho_{vac}(r) \approx -\frac{\alpha}{6\pi^2}\frac{Ze}{r^3}. \tag{4.9}$$

It is easy to show that this quantity is determined mainly by the contribution of the continuous spectrum in formula (4.4), and that the effective region of integration with respect to p extends to $p \sim 1/r \gg 1$. Therefore at $r \ll 1$ the contribution of the discrete spectrum (where $|p| = \sqrt{1 - \epsilon^2} \leq 1$) to $\rho_{vac}(r)$ can be neglected.

Expression (4.6) for the additional potential $\delta\varphi$ leads to a shift of the s-levels of hydrogen-like atoms; this shift is equal to (at $\zeta = Z\alpha \ll 1$)

$$\Delta E''_{nl} = \langle nl\,|\,\delta\varphi\,|\,nl\rangle = -\frac{4\alpha\zeta^4}{15n^3}\,\delta_{l0}. \tag{4.10}$$

In the nonrelativistic approximation the Uehling potential exerts an influence only on the s-states; in particular, it lowers the $2S_{1/2}$ level of the hydrogen atom by 1.1×10^{-8} eV = 27 MHz in comparison with the $2P_{1/2}$ level. This shift amounts to ~3% of the main part of the radiative corrections $\Delta E'_{nl}$, due to the interaction of the electron with the photon vacuum, where $\Delta E'_{nl}$ and $\Delta E''_{nl}$ have opposite signs (the total shift of the levels $2S_{1/2}$ and $2P_{1/2}$ in hydrogen is equal to $\Delta E = \Delta E' + \Delta E'' = 1058$ MHz). Since the theory agrees presently with experiment to within 0.15 MHz (see [62]), this is direct evidence that vacuum-polarization effects are real and are correctly described by the theory.*

4.2. Let us turn now to a situation arising when $\zeta = Z\alpha > 1$ and the charge of the nucleus Z passes through the critical value Z_c. Assuming

$$\rho_\epsilon(r) = |g_\epsilon(r)|^2 + |f_\epsilon(r)|^2,$$

where $g_\epsilon(r)$ and $f_\epsilon(r)$ are radial functions for the energy ϵ, we have

$$\rho_{vac}(r) = \frac{e}{2}\left\{\sum_{-1<\varepsilon_n<1}\rho_n(r) + \int\limits_0^\infty dp\,[\rho_\varepsilon(r) - \rho_{-\varepsilon}(r)]\right\}. \tag{4.11}$$

It will be convenient for us to denote the quantities pertaining to the cases $Z < Z_c$ and $Z > Z_c$ by the indices − and +, respectively. At $Z \sim Z_c$, abrupt changes are experienced only by wave functions with energy close to −1, namely:

*See [15]; for a short-range potential (square well) the polarization of vacuum is considered in a recent paper [61].

*We note here that expression (4.10) for $\Delta E''_{nl}$ can be obtained also without using the exact formula (4.6) for the Uehling potential. To this end it suffices to take into account the first term of the series in (1.5), $\delta\varphi(r) = -(\alpha/15\pi m_e^2)\Delta\varphi_0$, which in the case of a Coulomb potential $\varphi_0(r) = Ze/r$ yields $\delta\varphi(r) = (4\alpha Ze/m_e^2)\delta(r)$. At $Z\alpha \ll 1$, this expression for $\delta\varphi$ is equivalent to (4.6) in the sense that both give the same value for $\Delta E''_{nl}$. The replacement of (4.6) by a δ function is possible because the Uehling potential is short-range (compared with the Bohr radius). In other cases, when the average radius of the state is comparable with $\hbar/m_e c$, it is necessary to use formula (4.6) (this is the situation, for example, in the case of μ-mesic atoms [63,64]).

1) At $Z < Z_c$ the sum over the states of discrete spectrum contains a term $\rho_1(r)$ corresponding to the level 1S, and at $Z > Z_c$ this term vanishes from the complete set of the single-particle functions.

2) On the other hand, when $Z > Z_c$, the lower-continuum functions with angular momentum $j = 1/2$ experience strong perturbations (they increase sharply at small r); this perturbation is quantitatively described by the formula*

$$\rho_\varepsilon^+(r) - \rho_\varepsilon^-(r) \approx \Delta(p)\,\rho_c(r); \qquad (4.12)$$

here $\Delta(p)$ is given by (3.13), $p = \sqrt{\epsilon^2 - 1}$, and $\rho_c(r) = |g_c|^2 + |f_c|^2$ is the square of the wave function at $Z = Z_c$ and $\epsilon = -1$ (see formula (2.22)).

For all the remaining states, the point $Z = Z_c$ is not distinguished in any way, and these states produce in $\rho_{vac}(r)$ a background that varies slowly with $Z - Z_c$.

Thus, the change of ρ_{vac} on going through Z_c is equal to

$$\rho_{vac}^+(r) - \rho_{vac}^-(r) = -\frac{e}{2}\left[2\rho_c(r) + 2\int_0^\infty dp\,\Delta(p)\,\rho_c(r)\right] = -2e\rho_c(r)$$

(the factor 2 takes into account the double degeneracy with respect to the spin projection).

When $Z > Z_c$, the vacuum becomes charged. The total charge of the vacuum is equal to $-2e$, and therefore for an external observer the effective charge of the nucleus Z decreases to $Z - 2$. If we have at $Z < Z_c$ an uncharged vacuum (a bare nucleus whose 1S level is not occupied by electrons), then spontaneous emission of two positrons occurs when several protons are added to the nucleus, and the vacuum acquires two units of negative charge in accord with the electric-charge conservation law.

To avoid misunderstandings, let us make a stipulation with respect to the term "charged vacuum." When $Z > Z_c$, as well as when $Z < Z_c$, we define as the vacuum the lowest energy state* in the field of a nucleus with charge Z. So long as $Z < Z_c$, it corresponds to a bare nucleus with unfilled shells. On going through $Z = Z_c$, the bare nucleus becomes metastable and a realignment of the vacuum takes place (by emission of two positrons). The instability of the "old" vacuum at $Z > Z_c$ is due to the fact that three curves $\epsilon = \epsilon_i(Z)$, $i = 0, 1, 2$, intersect at the point $Z = Z_c$ ($i = 0$ corresponds to the energy of the vacuum at $Z < Z_c$, and $i = 1$ and 2 correspond to the energies of the states with one and two pairs, respectively).

When $Z > Z_c$, the $\epsilon_2(Z)$ curve goes below the $\epsilon_0(Z)$ and $\epsilon_1(Z)$ curves. The additional charge density $\rho_0(r) = \rho_{vac}^+(r) - \rho_{vac}^-(r)$, which occurs in the vacuum when Z goes through Z_c, gives the mathematical description of the K shell in the supercritical atom (see Sec. 1). We note that the approximations (4.12) and (4.13) are valid only at $(Z - Z_c) \ll Z_c$. In principle, however, the use of formula (4.11) with exact Coulomb functions makes it possible to find the charge density $\rho_0(r)$ of the K shell also at larger values of $Z - Z_c$.

The charge density $\rho_{vac}(r)$ at $r \ll 1$ is determined mainly by the contribution of the states of the continuous spectrum with $p \gtrsim 1/r \gg 1$, which are insensitive to $Z - Z_c$. Consequently, the polarization of the vacuum at small distances does not experience any changes at the point $Z = Z_c$. On the other hand, at $r \gg 1$, the initial Coulomb field is small ($E(r) \ll E_c = m_e^2c^3/e\hbar$), as the result of which the polarization of the vacuum attenuates exponentially (see (4.7)). The entire change of the charge of the vacuum at the point $Z = Z_c$ is distributed in space in the same manner as $\rho_c(r)$, i.e., is localized in the region $r \sim 1$ (see Figs. 3 and 9).

Thus, were it possible to combine (at least temporarily) two bare uranium nuclei and produce a nucleus with supercritical $Z = 184 > Z_c$, then one could expect spontaneous emission of two positrons to occur. Their kinetic energy at infinity is proportional to $Z - Z_c$ (so long as $(Z - Z_c) \ll Z_c$) and tends to zero as $Z \to Z_c$.

The threshold behavior of the probability of positron production w is determined by the Coulomb barrier. Apart from a pre-exponential factor, w coincides with the penetrability of the barrier:

$$w \sim \frac{m_e c^2}{\hbar}\exp(-2\pi\zeta_c/p), \qquad (4.14)$$

where $p = \sqrt{\epsilon^2 - 1}$ is the momentum of the emitted positrons (it is assumed that $p \ll 1$). When the nuclear charge Z exceeds Z_c only slightly, the resonance $E = \epsilon_0 - (i\gamma/2)$ is extremely narrow and practically all the positrons are emitted with the same energy:

$$\varepsilon = -\varepsilon_0 = 1 + \beta(\zeta - \zeta_c), \quad p = \sqrt{\varepsilon_0^2 - 1} \text{ where } \beta = -\left(\frac{\partial\varepsilon}{\partial\zeta}\right)_{\zeta=\zeta_c}.$$

In this case the exponential in w can be represented in the form[11]

$$w \sim \exp\left(-b\sqrt{\frac{Z_c}{Z - Z_c}}\right), \quad b = 2\pi\sqrt{\frac{\zeta_c}{2\beta}}. \qquad (4.15)$$

In the approximation $\Lambda \gg 1$ we have $\beta = 3\Lambda^3/5\pi^2$ and $b = 18\Lambda^{-3/2}$ ($\Lambda = -\ln R$). In the real region $R \sim 10^{-12}$ cm, this asymptotic formula for the coefficient b is inaccurate, and a numerical calculation is necessary. The results of such a calculation are shown in Fig. 13 for the simplest model of a rectangular cutoff of the potential inside the nucleus (the dependence of b on the form of the cutoff of V(r) at $r < R$ is quite weak).

For $Z_c = 170$ we find $b = 1.73$, so that at $Z = Z_c + 1$ the exponential in (4.15) is of the order of 10^{-10}. The strong dependence of w on the excess of the charge Z over Z_c can be seen from the fact that the w increases by three orders of magnitude on going from $Z = Z_c + 1$ to $Z = Z_c + 2$.

We note also the following fact: at the instant ($Z = Z_c' = 185$) when the $2P_{1/2}$ level reaches the boundary of the continuum $\epsilon = -1$, the first level of $1S_{1/2}$ penetrates

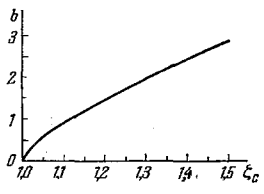

FIG. 13. The coefficient b in formula (4.15) as a function of $\zeta_c = Z_c/137$.

*We note that the perturbation $\rho^+ - \rho_\epsilon^-$ is well localized in space. On the other hand, neither of the functions $\rho_\epsilon^\pm(r)$ tends to zero as $r \to \infty$, since $g_\epsilon(r)$ and $f_\epsilon(r)$ are states of the continuous spectrum. All that is localized is the difference $\rho_\epsilon^+(r) - \rho_\epsilon^-(r)$ integrated over the continuous spectrum.

*Among the states having a total charge Z (with allowance for the particles that go off to infinity).

deeper into the lower continuum by an amount $|1 + \epsilon_0| \sim m_e c^2$, which is comparable with the height of the barrier in (2.16). The probability w(1S) then ceases to be exponentially small.

4.3. The positron production process can be described in greater detail by turning to some concrete formulation of the experiment whereby $Z > Z_c$ is obtained, for example in the collision of two heavy nuclei.[9,65] If v_0 is the velocity of the nuclei at infinity and R is the distance of their closest approach, then $Mv_0^2 = (Ze)^2/R$, whence

$$v_0 = \sqrt{\frac{Z}{A}\frac{m_e}{m_p}\frac{\zeta}{R}} = \frac{1}{70}\sqrt{\frac{\zeta}{R}} \qquad (4.16)$$

($\zeta = Z/137$ and R is measured in units of $\hbar/m_e c$). At $\zeta \approx {}^2/_3$ (for uranium nuclei) and $R > 0.1$ we have $v_0 < 0.03$, i.e., the motion of the nuclei can be regarded as nonrelativistic.

The characteristic collision time is

$$\tau_c = R/v_0 = 70\zeta^{-1/2}R^{3/2}, \qquad (4.17)$$

where $\tau_c \gg 1$ at $R > 0.1$. For motion of a bound electron in an internal well ($r < r_0$) the period is $\tau_0 \sim \bar{r}/\bar{v}$; as $\epsilon \to -1$ we have $\bar{r} = 0.3$, $\bar{v} = 1$ (the state does not become delocalized), and therefore $\tau_c \gg \tau_0$. Consequently, the electron energy levels can be determined in the adiabatic approximation by considering the coming together of the nuclei as a quasistatic process. This gives the same curve $\epsilon = \epsilon(R)$ as for nuclei at rest.

When two nuclei with charge $Z < Z_c$ each come together until the distance between them is $R < 1$, a field is produced, which for electron differs little from the field of a point-like charge 2Z, although the nuclei have by far not yet coalesced. We shall assume that the (bare) nuclei have come together a distance such that the lower level of the electron acquires an energy* $\epsilon_1(R) < -1$. At the instant when $\epsilon_1 = -1$, this (unfilled) level corresponds to two holes in the lower continuum, i.e., to two positrons. Owing to the Coulomb barrier in the effective potential U, these positrons are localized near the nucleus (their wave function is close to (2.22)).

In principle, the given positron-production mechanism is not connected in any way with the frequency of the electric field $\omega_c \sim 1/\tau_c$, and is possible when the nuclei approach each other very slowly. We estimate the number of produced positrons n_p by starting from the formula $\dot{n} = -\gamma(t)n$, where $n = n(t)$ is the number of bare nuclei at the instant t, and $\gamma(t)$ is the instantaneous probability of positron emission (corresponding to a distance R(t) between nuclei). Hence

$$\frac{n_p}{n(-\infty)} = 1 - \exp\left\{-\int_{-\infty}^{\infty}\gamma(t)\,dt\right\}. \qquad (4.18)$$

So long as the excess of the effective charge $Z_{eff} = Z_{eff}(R)$ over Z_c is small, we have $n_p = w_1 n(-\infty)$, where $w_1 = \int\gamma(t)dt \ll 1$. The probabilities of production of one pair (w_1) and of two pairs (w_2) in this case are as follows: $w_2 \sim w_1^2 \ll w_1 \ll 1$. The positrons are produced mainly at the instant of the closest approach of the nuclei and have an energy very close to the energy of the level $\epsilon_0(R)$ at the closest approach.*

Table I

R		I			II	
F	in units of $\hbar/m_e c$	$1S_{1/2}$	$2P_{1/2}$	$2S_{1/2}$	$1S_{1/2}$	$2P_{1/2}$
8	0.0207	1.248	1.35	1.72	1.224	1.31
10	0.0259	1.271	1.38	1.78	1.243	1.34
12	0.0311	1.291	1.41	1.83	1.260	1.365

Columns I and II pertain to two cutoff models in formula (2.5): I) f(x) = 1, charge on the surface of the nucleus; II) uniform distribution of charge over the volume of the nucleus.

With further increase of Z_{eff} (or, equivalently, with decreasing R), an instant sets in when $\int\gamma(t)dt \sim 1$ (this occurs when the 1S level deepens into the lower continuum by an amount $\sim m_e c^2$, comparable with the height of the Coulomb barrier). Here $w_2 \sim 1$, i.e., practically all the nuclei produce two positrons each. This concludes the process of positron production as a result of the 1S level.† Positron production becomes possible again only at values of R such that the boundary $\epsilon = -1$ is crossed by the following levels: $2P_{1/2}$, $2S_{1/2}$, $3P_{1/2}$, etc. To this end, just as in the case of one nucleus of radius R, it is necessary to have an appreciable increase of Z_{eff} (see Table I, which gives the values of $\zeta_c = Z_c 137$ for the first three levels).

When the nuclei move apart, the electrons remain as a rule bound on the moving nuclei with $Z < Z_c$. On these nuclei, the binding energies are lower, since $\epsilon_1(Z) > -1$. There is apparently little likelihood that the process will return adiabatically in the direction of the pair annihilation with increasing distance between nuclei. It is easy to see that the overall energy balance is not violated: on the whole, the energy necessary for pair production is drawn from the kinetic energy of the nuclei. As a result of the smaller charge (Z − 1), the nuclei move apart with a kinetic energy lower than the initial one.

In a more accurate calculation of the probability w_1 and w_2, of the momentum spectrum of the positrons, etc., it is necessary to consider the dynamics of tunneling of the positron with allowance for the finite velocity of the nuclei.‡ Such calculations can be carried out by using, for example, the method of imaginary time in subbarrier motion (see [87] and also [22], p. 225); they will

*For quantitative predictions it is necessary to know the dependence of Z_c on R for the two-center problem. In the relativistic case, the variables in it do not separate, but the value of $Z_c(R)$ can be found by a variational method [65]. Such calculations are presently being carried out; preliminary results were published in [66].

*Here ϵ_0 is the real part of the Breit-Wigner pole $E = \epsilon_0 - (i\gamma/2)$, which is an analytic continuation (see the preceding section) of the 1S level at $Z > Z_c$.

†The average positron energy $\bar{\epsilon}$ is determined by the position of the resonant level $\epsilon_0(R)$ for a distance R such that $\int\gamma(t)dt \sim 1$. As the nuclei come closer together, when $\int\gamma(t)dt$ becomes much greater than 1, the positrons are no longer produced in practice and the energy ϵ remains unchanged.

‡The time of tunneling through the Coulomb barrier $U(r) = \zeta/r$ is equal to $\tau_t = \int_0^{r_0} dr|p(r)|^{-1/2} = \pi\zeta p^{-3}$, where $r_0 = 2\zeta/p^2$ is the turning point and p is the momentum of the positron at infinity. As $p \to 0$, the tunneling time is very large. Comparison of τ_t with τ_c (see (4.17)) shows that the tunneling process can be regarded as adiabatic at $p \gtrsim v_0$, where v_0 is the velocity of the nuclei at infinity.

Table II

R	ω_c
1	0.012
0.5	0.033
0.1	0.37

become necessary when the corresponding experimental data become available.

The process competing with that considered above is pair production as a result of the frequency of the variation of the electric field or via excitation of the nuclei upon collision. However, owing to the large mass of the nuclei, their motion (at not too small values of R) is so much slower that pair production as a result of the Fourier components of the electric field with frequency $\omega > 2m_e$ will be negligibly small (see Table II, which shows the values of the frequency $\omega_c = 1/\tau_c$ in units of $m_e c^2$ for $\zeta = 2/3$, corresponding to collision of uranium nuclei; R is the shortest distance between the nuclei in units $\hbar/m_e c$; τ_c is the characteristic collision time (see (4.17)). In principle, this makes it possible to separate the quasistatic mechanism of positron production (as a result of the excess of the summary charge 2Z over Z_c) from other possible mechanisms.

4.4. So far we have considered bare nuclei. If the level 1S is filled with electrons, then on going through $Z = Z_c$ no visible effects will occur. The electron cloud, carrying a charge $-2e$, is produced at $Z < Z_c$ by two electrons at the lower (discrete) level, and at $Z > Z_c$ it is produced by perturbation of the functions of the continuum near the energy $\epsilon = \epsilon_0 < -1$. If we integrate the charge density over the entire continuous spectrum, then at $Z > Z_c$ we obtain (after renormalization) precisely an excess charge $-2e$. Although formally the K shell has vanished at $Z > Z_c$ (owing to the single-particle solutions of the Dirac equation), its role is assumed by the continuous spectrum. Therefore, for example, the electrons of the outer shells of the atom experience no change whatever at the point $Z = Z_c$ in this case.

Of course, the K shell in the supercritical atom has certain peculiarities compared with the K shell in the ordinary atom with $Z < Z_c$.

However, these differences are not connected with the jump in the average radius of the K shell or with the sharp change of the density of the electric charge, and are more subtle (e.g., there is a resonance in the scattering of the positrons by an atom with $Z > Z_c$; see Sec. 1 concerning this subject).

In conclusion we note that the question of production of pairs of particles and antiparticles under the influence of a strong field has recently become very urgent in cosmology. Preliminary estimates show that pair production may substantially influence the evolution of the universe near a singularity.[68,69]

5. PROPERTIES OF RELATIVISTIC WAVE EQUATIONS WITH POTENTIAL

In this section we discuss briefly the motion of levels with increasing depth of potential for other relativistic equations. As is well known, in the case of free particles the entire mathematical formalism of quantum theory (wave equations, Green's function, Feynman diagrams, etc.) can be developed quite consistently for particles having any spin (see [70-74], where further references can be found). When a (sufficiently strong) potential is turned on, however, the situation changes.*

5.1. We start with the case of a scalar (spinless) particle. The Klein-Gordon equation with vector coupling

$$\Delta\varphi + [(\varepsilon - V)^2 - 1]\varphi = 0 \tag{5.1}$$

is formally equivalent to the nonrelativistic Schrödinger equation $\chi'' + 2(E - U)\chi = 0$, where

$$E = \frac{\varepsilon^2 - 1}{2}, \quad U = \varepsilon V - \frac{1}{2}V^2 + \frac{l(l+1)}{2r^2}. \tag{5.2}$$

However, the fact that the energy ϵ enters in (5.1) quadratically, changes the form of the orthogonality condition:

$$\int d^3r \varphi_\lambda^*(\mathbf{r})\{\varepsilon_\lambda + \varepsilon_{\lambda'} - 2V(r)\}\varphi_{\lambda'}(\mathbf{r}) = \eta_\lambda \delta_{\lambda\lambda'}; \tag{5.3}$$

here $\varphi_\lambda(\mathbf{r})$ and $\varphi_{\lambda'}(\mathbf{r})$ are the wave functions of the discrete spectrum ($-1 < \epsilon_\lambda, \epsilon_{\lambda'} < 1$), and $\eta_\lambda = \pm 1$. For levels going from the upper continuum $\eta_\lambda = 1$, and for levels going from the lower continuum we must put $\eta_\lambda = -1$ (the validity of this statement becomes obvious if V(r) is excluded).

Unlike the Dirac case, the dependence of ϵ on V is not monotonic here, and the curve $\epsilon = \epsilon(V)$ can have an inflection. This phenomenon was observed in [75] with s-states in a square well as an example.

Let us consider it in greater detail, without confining ourselves to the case $l = 0$. We put

$$V(r) = -v\theta(r_0 - r), \qquad v > 0 \tag{5.4}$$

(r_0 is the radius of the well; the depth of the well v is measured in units of mc^2). The wave function $\chi_l(r)$ has the same form as in the nonrelativistic problem:

$$\chi_l(r) = \begin{cases} \sqrt{r}\, J_{l+1/2}(kr), & r < r_0, \\ \sqrt{r}\, K_{l+1/2}(\lambda r), & r > r_0, \end{cases} \tag{5.5}$$

differing only in the values of the parameters k and λ:

$$k = [(\varepsilon + v)^2 - 1]^{1/2}, \quad \lambda = (1 - \varepsilon^2)^{1/2}.$$

From the condition for matching at $r = r_0$ we obtain an equation for the level energy ϵ

$$k\frac{J_{l-1/2}(kr_0)}{J_{l+1/2}(kr_0)} = -\lambda\frac{K_{l-1/2}(\lambda r_0)}{K_{l+1/2}(\lambda r_0)}. \tag{5.6}$$

λ vanishes at $\epsilon = \pm 1$ and Eq, (5.6) simplifies

$$J_{l-1/2}(\xi) = 0, \tag{5.7}$$

where $\xi = k_\pm r_0$ and $k_\pm = \sqrt{v^2 \pm 2v}$ for $\epsilon = \pm 1$.

Let ξ_l the smallest possible root of (5.7): $\xi_0 = \pi/2$, $\xi_1 = \pi$, $\xi_2 = 1.42\pi, \ldots$; the ξ_l increases with l. Then at the instant when the first level with orbital angular momentum l appears the depth of the well is (for $\epsilon = \pm 1$)

$$v_l^\pm = \sqrt{1 + (\xi_l/r_0)^2} \mp 1. \tag{5.8}$$

*The electromagnetic interaction is introduced in minimal fashion ($\partial_\mu \to \partial_\mu - ieA_\mu$). The potential V(r) is regarded everywhere as the temporal component of the 4-vector $A_\mu(x)$: $\mathbf{A} = 0$, $V(r) = eA_0$. In addition, we put $m = 1$, where m is the mass of a particle moving in a field V(r).

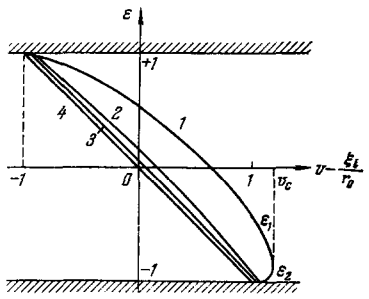

FIG. 14. Levels of scalar particle in a narrow well ($r_0 = 0.3\hbar/mc$) as a function of the depth v of the well. The abscissas represent $v-(\xi_l/r_0)$. Curves 1–4 correspond to the cases $l = 0$, 1, 2, and $l \gg 1$.

In the case of broad well ($r_0 \gg \hbar/mc = 1$) we have $v_l^+ = \xi_l^2/2r_0^2$ and $v_l^- = 2 + \xi_l^2/2r_0^2$, and for a narrow well ($r_0 \ll 1$) we have $v_l^\pm = \xi_l/r_0 \mp 1 + O(r_0)$. In the case of a narrow well it is easy to determine not only the values of $v_l^\pm$, but also the entire $\epsilon = \epsilon(v)$ curve. Expanding (5.6) in powers of r_0, we obtain

$$v = v(\varepsilon) = \begin{cases} \frac{\pi}{2r_0} + \frac{2}{\pi}\sqrt{1-\varepsilon^2} - \varepsilon + \left[1 - \frac{8}{\pi^2}(1-\varepsilon^2)\right]\frac{r_0}{\pi} + \ldots & \text{for } l = 0, \\ \frac{\xi_l}{r_0} - \varepsilon + \frac{l+1/2-\varepsilon^2}{(2l-1)\xi_l} r_0 + \ldots & \text{for } l \gg 1. \end{cases} \tag{5.9}$$

As see from Fig. 14, the $\epsilon = \epsilon(v)$ curve for the s-states turns out to have an inflection, and at $l \geq 1$ the energy ϵ decreases monotonically with increasing v. These conclusions remain in force also for a broad well, but the inflection is in this case located very close to the boundary $\epsilon = -1$. The occurrence of the inflection of the curve $\epsilon = \epsilon(v)$ for the state with $l = 0$ is nothing peculiar for a potential in the form of a square well (5.4). As shown in [11], the same phenomenon takes place for the ground level in a short-range potential of any form. How is one to explain such a strange behavior of the s-level energy? At $v = v_-$ there appears in the well a bound state ϵ_2 (the lower branch of the curve 1 on Fig. 14). The physical interpretation of this state was indicated by Migdal,[25 53] namely, ϵ_2 is the level for the antiparticles (with potential $-V$), and not for particles. With further increase of v, a value $v = v_c$, corresponding to the vertex of the inflection, is reached.

At $v = v_c$ the levels ϵ_1 and ϵ_2 collide and go off to the complex plane. At $v > v_c$ we have two solutions with complex energies ϵ and $\bar{\epsilon}$, for which $\mathrm{Re}\,\lambda > 0$, and therefore the wave function (5.5) remains square-integrable. Thus, the single-particle Hamiltonian ceases to be a Hermitian operator at $v > v_c$. This is an indication that as $v \to v_c$ it is necessary in principle to take many-particle effects into consideration.*

The appearance of complex eigenvalues in a strong field is a rather common property of the Klein-Gordon equation. This can be seen from the formula of perturbation theory for the level shift. Putting in (5.1) $V = V_0 + \delta V$ and $\psi = \psi_0 + \delta\psi$, where $\psi_0(r)$ is a solution that decreases exponentially at infinity in the potential $V_0(r)$, we obtain the level shift

$$\delta\varepsilon = \frac{\varepsilon\overline{\delta V} - \overline{V}\overline{\delta V}}{\varepsilon - \overline{V}}. \tag{5.10}$$

The mean values ($\overline{V}$, $\overline{\delta V}$) are understood here in the usual sense:

$$\overline{V} = \int d^3r V(r)\,\varphi_0^2(\mathbf{r}) \Big/ \int d^3r \varphi_0^2(\mathbf{r}). \tag{5.11}$$

In the nonrelativistic limit as $\epsilon \to 1$ we have $\overline{V} \ll 1$, and expression (5.10) takes the usual form $\delta\epsilon = \overline{\delta V}$. On the other hand, in a deep well the condition $\epsilon = \overline{V}$ may be satisfied. At this point $\partial\epsilon/\partial V = \infty$, i.e., the level $\epsilon = \epsilon(V)$ has an inflection. With further deepening of V(r), the colliding branches ϵ_1 and ϵ_2 go over into a pair of states with complex-conjugate energies,* and $\mathrm{Re}\,\epsilon = V$. Since the corresponding poles of the S matrix lie on the physical sheet, we arrive at a contradiction to unitarity (meaning that the Hamiltonian is not hermetian).

For s-states there exists a centrifugal barrier in U(r), and if $\lim_{r\to\infty} r^2V(r) = 0$, then the wave function $\chi_\epsilon(r)$ becomes delocalized at $\epsilon \to \pm 1$. Therefore $\overline{V} = 0$ at the instant of occurrence of the level (the integral in the numerator of (5.11) converges and that in the denominator diverges). Thus $\epsilon - \overline{V}$ is equal to ± 1 on the edge of the upper and lower continuum, meaning that it vanishes at some intermediate point of the curve $\epsilon = \epsilon(V)$, which leads in accord with (5.10) to a collision of the two branches of the curve $\epsilon = \epsilon(V)$ and causes the energies ϵ_1 and ϵ_2 to go off to the complex plane.

We note that this reasoning is not valid when $l \geq 1$, since $\chi_l(r)$ remains normalizable at $\epsilon = \pm 1$ because of the centrifugal barrier (namely, at the instant of the appearance of the level $\chi_l(r) \sim r^{-l}$, $r \to \infty$). Therefore we can no longer state that $\overline{V} = 0$ at the edge of the continuum. This means a difference between the curves with $l = 0$ and $l \geq 1$ on Fig. 14. The same pertains also to the case of a Coulomb field, when the barrier in U(r) as $\epsilon \to -1$ is even more impenetrable. At $\epsilon = -1$ we have here $\epsilon - \overline{V} = 2 > 0$; there is no inflection, i.e., there is no large difference between the behavior of the level for scalar and spinor particles in an unscreened Coulomb field.[10,12]

5.2. We proceed to a spin $s = 1$. The question of the level spectrum of a vector particle in a Coulomb field has a history of 30 years behind it,[78,79] but it is still not fully clear. A mathematically correct formulation of this question is due to Case,[38] who showed that the roots of the difficulties arising here are the same as in the nonrelativistic problems with "falling to the center." In order to make the solution unique, it is necessary to choose a suitable boundary condition for small r.

By considering the Proca equation with potential V(r) that is singular at $r \to 0$, we can show[10,65] that the effective potential U acquires a stronger singularity (for states with angular momentum $j \geq 1$):

$$U(r) \underset{(r\to 0)}{\approx} -\frac{\sqrt{j(j+1)}}{2r}|V'(r)|. \tag{5.12}$$

*An attempt was made in [76,77] to consider a well with $v > v_c$ within the framework of the single-particle approximation, but the authors had to introduce an indefinite metric. As shown by Migdal [53], when $v > v_c$ there is virtual pair production and polarization of vacuum.

*From the conditions of generalized orthogonality (5.3) it does not follow now that the eigenvalues ϵ_λ are real (unlike the Dirac and Schrödinger equations), and all we get is the condition $\mathrm{Re}\,\epsilon_\lambda = \overline{V}$ for solutions with complex energy ($\mathrm{Im}\,\epsilon_\lambda \neq 0$).

In particular, the Coulomb case $V(r) = -\zeta/r$ corresponds to $U(r) \approx -\zeta\sqrt{j(j+1)}/2r^3$ (see [78]). The potential that serves as the limit between the regular and singular potentials is now V(r) with a singularity as weak as logarithmic: $V(r) = \zeta \ln r$. At sufficiently small ζ it is regular, and at $|\zeta|\sqrt{j(j+1)} > (j+1/2)^2$ it becomes singular and requires cutoff in the region of small r.

5.3. Equations for particles with higher spins ($s \geq 3/2$) were considered by many workers, starting with the classical papers of Fierz and Pauli[80] and Rarita and Schwinger.[81] It is difficult to introduce the electromagnetic field in these equations because it is necessary to ensure compatibility of the equations of motion with the additional conditions that exclude smaller spins. The customary procedure* consists of making the substitution $\partial_\mu \to \partial_\mu - ieA_\mu$ in the Lagrangian of the free field.[80] It was noted however only recently[82] that even in this case there is a discrepancy with relativity theory, namely, although the obtained equations are formally Lorentz-covariant, their solutions can propagate with superluminal velocity. This result is obtained from an analysis of the characteristics of the relativistic wave equations at $s \leq 3/2$. The parameter that determines the degree of violation of the causality is here the ratio H/H_0 or E/E_0, where $E_0 = H_0 = m^2c^3/e\hbar$, and m is the particle mass (the existence of electrons with $m_e < m$ is ignored in the theory). Although in such fields the quantum nonlinearities in the Lagrangian of the electromagnetic field already become significant, within the framework of the single-particle approach it is necessary to state that at present there are no good equations for the local field $\psi(x)$ with spin $s \geq 3/2$ (such equations can be written for the free field $\psi(x)$, but the difficulties indicated above arise in a sufficiently strong external electromagnetic field). Thus, the only relativistic equation for which the single-particle solutions in an external electric field V(r) remain meaningful at arbitrarily large |V| is the Dirac equation. On the other hand, it is precisely in this case that there are physical objects described by such equations (the light particles e^+ and $\mu^\pm$ in the field of a nucleus). It can be assumed that such a coincidence is not accidental.

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*Which makes it possible, in any case, to avoid direct algebraic contradictions, since both the equations of motion and the additional conditions are obtained by varying the Lagrangian L.

Notes added in proof. 1) It is reported in [83] that particles with $Z \sim 112$ have been registered. This discovery, if confirmed, will undoubtedly increase the interest in phenomena occurring at $Z > 137$. 2) The Lamb shift of levels in atoms with large Z (up to Z = 180) is estimated in [84]. Allowance for this shift raises the critical charge Z_c for the 1S level by approximately 5 units. 3) It is stated in [85,86] that the polarization of vacuum increases without limit as $Z \to Z_c$. This contradicts the conclusions of Chap. 4.

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