The Thomas-Fermi method for $Z > 137$

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A solution is obtained for the relativistic Thomas-Fermi equation for the electron cloud density near supercritical ($Ze^2 \gg 1$) nuclei. The cases of a vacuum ion (supercritical nucleus surrounded by a vacuum shell), neutral atom and positive ion are considered. The angular momentum distribution of the vacuum shell electrons is found. For $Ze^3 \ll 1$ (weak screening), the electron shell of the supercritical atom consists of two parts which almost do not overlap. These are the vacuum shell with a radius $r_0 \sim Ze^2/2$ and the outer shell with a radius $r_e \sim (Z^{1/3}e^2)^{-1}$. "Falling to the center" is investigated in the relativistic Thomas-Fermi equation. The nature of the singularities of the equation solutions as $r \to 0$ is determined by the renormalization group technique. A differential equation for the Gell-Mann–Low function $\beta(\mu)$ is obtained and its asymptotic values are found for $\mu \to 0$ and $\mu \to \infty$. A numerical solution is obtained for all values of the effective coupling constant μ.

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1. INTRODUCTION

The statistical Thomas-Fermi method is one of the most important methods of quantum-mechanical investigation of the many-body problem and is widely applied in atomic and molecular physics, astrophysics and so forth (see, for example, Refs. 1–3). The following Thomas-Fermi relativistic equation was obtained in Refs. 4 and 5:

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

and the electron density distribution

$$n_e(r) = \frac{1}{3\pi^2} (V^2 \pm 2V)^{3/2} \tag{2}$$

was found in the shell of a supercritical ($Ze^2 \gg 1$) ion. Here $V(r)$ is the self-consistent potential for the electron (in units of $m_e c^2$), and takes into account the screening action of the shell electrons, while $n_p(r)$ is the proton density in the nucleus.[1)] The upper sign in Eqs. (1) and (2) refers to the vacuum shell, which the bare nucleus with charge $Z > Z_{cr} \approx 170$ draws toward itself after spontaneous creation of e^+e^- pairs and flight of the positrons to infinity; the lower sign corresponds to the neutral atoms, in which not only the vacuum shells but also the outer electron shells are filled.

We now make a note concerning our terminology. We call (1) the "relativistic Thomas-Fermi equation," since it is a generalization of the usual[1–3] Thomas-Fermi equation to the case in which the potential $V(r)$ and the mean energy of the electrons of the atomic shell are equal to (or greater than) the rest mass $m_e c^2$. It is obvious that Eq. (1) is not relativistically invariant and refers to a selected system of coordinates in which the nucleus is at rest. A detailed derivation of Eq. (1) and a discussion of the exchange (Dirac type) and correlation corrections can be found in the Appendix to Ref. 5.

Only the vacuum shell of the supercritical atom was considered in Ref. 5. In the present work, we have continued the study of the relativistic Thomas-Fermi equation and treated the following problems:

1) The dependence of the "outer" charge of the ion $Z_1 = Z - N_e$ on the nuclear charge Z is found and the angular momentum distribution of electrons is calculated. Here N_e is the total number of electrons of the vacuum shell:

$$N_e = \int n_e(r) d^3r = \frac{4}{3\pi} \int_0^{r_a} (V^2 + 2V)^{3/2} r^2 \, dr, \tag{3}$$

r_a is its radius ($V(r_a) = -2$, see Ref. 5).

2) The electron shell of a neutral atom and a positive ion are considered at $Ze^2 \gg 1$. At $Ze^3 \lesssim 1$, the density of the electron gas $n_e(r)$ can be divided into two spatially separated parts: the vacuum shell, which is localized at distances $r \sim \hbar/m_e c = 1$ from the nucleus, and the outer electron shells, for which $r \sim 137 Z^{-1/3} \gg 1$.

3) The following results are developed in Sec. 5 in the study of the mathematical structure of Eq. (1): the character of the singularities that arise in the solutions of this equation at $r \to 0$ is described, and it is shown how the "falling to the center," which is characteristic for solutions of the Dirac equation at $\zeta > j + \frac{1}{2}$, enters into the many-electron problem.

In what follows, $\hbar = c = m_e = 1$, $\zeta = Ze^2 \approx Z/137$, $\zeta_{cr} = Z_{cr} e^2$ is the critical charge of the nucleus,[2)] $\varkappa = \mp(j + \frac{1}{2})$ for states with $j = l \pm \frac{1}{2}$. At $Ze^2 \gg 1$, we can neglect the diffuseness of the edge of the nucleus[5]; we therefore set

$$n_p(r) = n_p \theta(R - r) \tag{4}$$

in (1); here $R = r_0 A^{1/3}$ is the radius of the nucleus, $n_p = Zn_0/A$, $n_0 = 0.17$ F^{-3} is the density of nucleons in ordinary heavy nuclei.

2. VACUUM SHELL OF THE SUPERCRITICAL ION

The characteristic parameter in (1) is $Ze^3 \approx Z/1600$: at $Ze^3 \gtrsim 1$, the screening of the Coulomb potential of the nucleus by electrons becomes important. The vacuum-shell electron density was found[5] analytically in the limiting case $Ze^3 \ll 1$ and $Ze^3 \gg 1$, and numerically in the trsnsition region $Ze^3 \sim 1$. We denote by $Z_1 = Z - N_e$ the charge of the supercritical ion for an external ($r > r_a$)

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observer; at $r>r_a$, the density of the vacuum shell is equal to zero and the potential is $V(r)=-Z_1e^2/r$. Account of screening in the region $Ze^3 \ll 1$ is carried out by perturbation theory,[5] which yields

$$\frac{Z_1}{Z}=1-\frac{4}{3\pi}(Ze^3)^2\left(\ln\frac{\zeta}{R}+c_1\right) \tag{5}$$

(numerically, $c_1=-1.38$). In order to find Z_1 at arbitrary values of the parameter Ze^3, it is necessary to solve Eq. (1) with the boundary conditions

$$|V(0)|<\infty, \quad V'(0)=0; \quad V(r_a)=-r_aV'(r_a)=-2. \tag{6}$$

The joining of the inner and outer solutions at the edge of the nucleus determines the quantities Z_1, $r_a=Z_1e^2/2$, and $V(0)$. The results of the calculation of Z_1 are given in Fig. 1. The perturbation-theory formula (5) is applicable at $Ze^3<0.5$; in this region, the total charge of the vacuum shell is small in comparison with the charge of the nucleus.

In the opposite case $Ze^3 \gg 1$ (supercritical nuclei[12,13]), the quantity Z_1 at a fixed radius of the nucleus R takes on the limiting value $\overline{Z}_1=\overline{Z}_1(R)$, which depends on R (see Fig. 2). In the region of values of R that are characteristic for heavy nuclei, the quantity $\overline{Z}_1e^3$ is of the order of unity. The reason why the external charge of the ion remains bounded as $Z\to\infty$ is connected with "falling to the center" and is discussed in Sec. 5. At $Ze^3 \gtrsim 1$, the larger part of the electrons of the neutral atom belongs to the vacuum shell.

We now consider the angular-momentum distribution of the vacuum-shell electrons. The spatial density of electrons with angular momentum $j=|\varkappa|-\frac{1}{2}$ is of the form[5]

$$n_j(r)=\frac{|\varkappa|}{(\pi r)^2}\left[V^2+2V-\frac{\varkappa^2}{r^2}\right]^{1/2}. \tag{7}$$

The maximum angular momentum of the electrons of the vacuum shell $\varkappa_{max}$ first increases in proportion to Z; then this growth is slowed, $\varkappa_{max}\sim Z^{1/3}$ in the region $Ze^3 \gg 1$:

$$\varkappa_{max}=\max_{0<r<r_a} r(V^2+2V)^{1/2}=\begin{cases}\zeta-R, & Ze^3\ll 1\\ c\zeta(Ze^3)^{-2/3}, & Ze^3\gg 1\end{cases}, \tag{8}$$

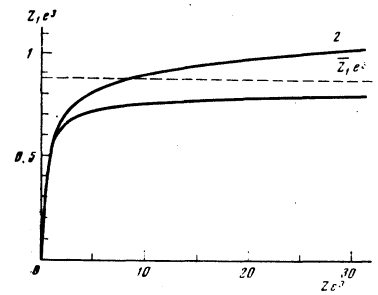

FIG. 1. The outer charge of the supercritical atom $Z_1=Z-N_e$ as a function of the nuclear charge Z. Curve 1 corresponds to a nucleus with density (4) and constant radius $R=0.03=11.6$ F, curve 2 is the usual dependence $R=r_0A^{1/3}$ ($r_0=1.1$ F, $A=2Z$). As $Z\to\infty$, curve 1 goes over to the limiting value, equal to $Z_1e^3=0.88$.

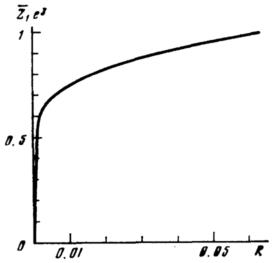

FIG. 2. Dependence of Z_1e^3 on the radius of the nucleus (the values of R are given in units of $\hbar/m_ec=386$ F).

where $c=(3/4)(9\pi/4)^{1/3}=1.44$.

At $Ze^3 \ll 1$, we can neglect the distortion of the potential of the nucleus due to screening, and assume[3)]

$$V(r)=\begin{cases}-\zeta/r, & r>R\\ -(\zeta/R)f(r/R), & 0<r<R\end{cases}. \tag{9}$$

Hence

$$n_j(r)=\frac{\zeta^2\rho}{\pi}\cdot\begin{cases}[(1-\rho^2)(1-r/r_1)]^{1/2}r^{-3}, & R<r<r_1\\ [f^2(x)-\rho^2/x^2]^{1/2}R^{-1}r^{-2}, & r_0<r<R\end{cases}, \tag{10}$$

where $\rho=|\varkappa|/\zeta$ ($0<\rho<1$), $x=r/R$, and r_0 and r_1 are the quasiclassical turning points: $r_0=Rx_0(\rho)$, where $x_0(\rho)$ is the root of the equation $xf(x)=\rho$, $r_1=(\zeta^2-\varkappa^2)/2\zeta=\zeta(1-\rho^2)/2$. Integrating (10) over d^3r, we find the angular-momentum distribution of the electrons:

$$n_j=(2\zeta/\pi)(1-\rho^2)^{1/2}[2(\mathrm{Arth}\sqrt{1-\eta}-\sqrt{1-\eta})+h(\rho)], \tag{11}$$

where $\eta=R/r_1=2R/\zeta(1-\rho^2)$ and the function $h(\rho)$ depends on the cutoff model:

$$h(\rho)=(1-\rho^2)^{-1/2}\int_{x_0(\rho)}^{1}[f^2(x)-\rho^2x^{-2}]^{1/2}dx.$$

Figure 3 shows (curve 1) the distribution (11) normalized by the condition

$$\int_0^1 n(\rho)d\rho=1;$$

here $n(\rho)$ differs from n_j only by the normalization constant. The density distribution $n(\rho)$ is practically inde-

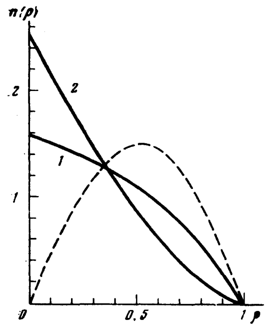

FIG. 3. Angular momentum distribution of the electrons of the vacuum shell ($\rho=|\varkappa|/\varkappa_{max}$). Curves 1 and 2 correspond to the two limiting cases $Z_e^3\ll 1$ and $Z_e^3\gg 1$; the dashed line shows the angular momentum distribution of the electrons ($\rho=l/l_{max}$) in the nonrelativistic Thomas-Fermi model.

pendent of the cutoff model (the curves for models I and II are identical within the limits of accuracy of the drawing). To explain this fact, we note that at $\varkappa$ not very close to $\varkappa_{max}$ we have $\eta \ll 1$ and the formula (11) can be rewritten in the form

$$n_j = \frac{2\zeta}{\pi}(1-\rho^2)^{1/2}\left[\ln\frac{\zeta}{R} + h_1(\rho)\right],$$
$$h_1(\rho) = h(\rho) + \ln(1-\rho^2) + \ln 2 - 2. \qquad (11')$$

The principal term in (11′), which contains the large logarithm $\ln(\zeta/R) \gg 1$, comes from the external region $r > R$, in which a purely Coulomb field is acting. The function $h_1(\rho)$, which is numerically small, depends on the specific form of the cutoff. Thus, the value

$$h_1(0) = \int_0^1 f(x)\,dx + \ln 2 - 2$$

is equal to -0.31 and 2.7×10^{-2}, respectively, for the cutoff models I and II.

In the case $Ze^3 \gg 1$, the potential inside the nucleus takes on a constant value[4,5]: $V(r) = -(3\pi^2 n_p)^{1/2}$ at $r < R$. Neglecting the diffuseness of the boundary, we find

$$n(\rho) = \frac{8}{\pi}\left[(1-\rho^2)^{1/2} - \rho \arccos\rho\right] \qquad (12)$$

—see the curve 2 in Fig. 3. The dashed curve in this same drawing shows the distribution of $n(\rho)$ in the shell of the neutral atom for the non-relativistic Thomas-Fermi model.[1] A comparison of it with curves 1 and 2 shows that in the vacuum shell of a supercritical atom, the fraction of electrons with angular momenta $|\varkappa| \ll \varkappa_{max}$ increases significantly.

The expressions (1)–(3) and the subsequent formulas are based on the quasiclassical approximation. The condition of their applicability to the Coulomb field in the relativistic case is[5,11] $(\zeta^2 - \varkappa^2)^{1/2} \gg 1$, or $1 - \rho \gg \zeta^{-2}$. The condition of quasiclassicality is violated only in a narrow range of angular momenta, near $\varkappa_{max}$. Because of the specific nature of the Coulomb field, the results obtained above have excellent accuracy, not only at $\zeta \gg 1$, but even for small values of ζ. Thus, the quasiclassical formula (3) is in excellent agreement with the numerical calculations of N_e in comparison with the Dirac equation,[11] beginning even at $\zeta = 2$.

3. THE NEUTRAL ATOM AT $Ze^2 \gg 1$

We now consider a neutral atom in which, in addition to the vacuum shell, the outer electron shells are filled (the corresponding levels have energies ε_n in the region of the discrete spectrum: $-1 < \varepsilon_n < 1$). Since the radius of the vacuum shell is $r_a \sim Ze^2$, and the mean radius of the atom in the nonrelativistic Thomas-Fermi model is $r_e \sim (Z^{1/3}e^2)^{-1}$, we have

$$r_a/r_e \sim (Ze^3)^{4/3}.$$

Therefore, in the case of weak screening ($Ze^3 \ll 1$), to which we limit ourselves, these two shells (vacuum and outer) are localized in different regions of space and almost do not overlap. While the electrons of the vacuum shell are completely relativistic, the outer shell consists mainly of nonrelativistic electrons (their mean energy is $\bar{\varepsilon}_n \sim m(Ze^3)^{4/3} \ll m$). This simplifies the problem and enables us to obtain a solution in analytic form.

The self-consistent potential for the neutral atom is described by Eq. (1) with a minus sign. Outside the nucleus,

$$\frac{d^2V}{dr^2} + \frac{2}{r}\frac{dV}{dr} = -\frac{4e^2}{3\pi}(V^2 - 2V)^{3/2}. \qquad (13)$$

The presence of the small parameter e^2 allows us to seek a solution by means of perturbation theory, which yields

$$V(r) = -\frac{\zeta}{r}\left[1 + \frac{4}{3\pi}(Ze^3)^2\{F(x) - a_1x - a_2\}\right], \qquad (14)$$

where $x = 2r/\zeta$; a_1 and a_2 are constants of integration,

$$F(x) = (2-3x)\,\mathrm{Arcth}\,(1+x)^{1/2} - 5(1+x)^{1/2} + {}^4/_3(1+x)^{3/2}$$
$$= \begin{cases} -\ln x + (2\ln 2 - {}^{11}/_3) + O(x\ln x), & x\to0 \\ {}^4/_3 x^{3/2} - 6x^{1/2} + O(x^{-1/2}), & x\to\infty \end{cases}. \qquad (15)$$

Inside the nucleus, Eq. (1) is solved with the boundary condition $V'(0) = 0$, which assures regularity at the zero. The joining of the inner ($r < R$) solution with (14) on the edge of the nucleus gives the relations

$$a_2 = \ln\frac{\zeta}{R} + \int_0^1 f^3(x')x'^2\,dx' + \ln 2 - {}^8/_3, \qquad (16)$$

$$V(0) = -\frac{\zeta}{R}f(0)\left[1 - \frac{8}{9\pi}(Ze^3)^2\left(1 + \int_0^1 f^3(x')x'\,dx'\right)\right] + \frac{8}{3\pi}a_1(Ze^3)^2 \qquad (17)$$

(here $x' = x/R$, and $f(x')$ is the cutoff function introduced in (9)).

For determination of the constant a_1, we consider the region $r \gg r_a$, in which $x \gg 1$, $|V(r)| \ll 1$ and Eq. (13) goes over into the nonrelativistic Thomas-Fermi equation for the function $\chi(y)$:

$$V(r) = -\frac{Z_1e^2}{r}\chi(y), \quad y = \frac{rZ_1^{1/3}}{b}, \quad b = \left(\frac{9\pi^2}{128}\right)^{1/3}\frac{1}{e^2}. \qquad (18)$$

In the region $r_a \ll r \ll r_e$, we have $y \ll 1$; therefore,[1,2] $\chi(y) = 1 - \gamma y + (4/3)y^{3/2} + \ldots$, where $\gamma = 1.588$; on the other hand, $x \gg 1$ and in (14) we can use the asymptotic form of $F(x)$ as $x \to \infty$. The joining of these solutions determines a_1:

$$a_1 = (3\pi/4)^{1/3}\gamma(Ze^3)^{-2/3}, \qquad (19)$$

which completes the solution of the problem.

4. POSITIVE ION

Like ordinary ($Ze^3 \ll 1$) atoms, the supercritical atom can be in an ionized state if the outer shell is partially filled. Such a state is stable for the isolated atom. Let $q = (Z - N)/Z$ be the degree of ionization: a neutral atom corresponds to $q = 0$, and the nucleus with the vacuum shell to $q = \bar{q} \equiv (Z - N_e)/Z$. The $\bar{q}(Z)$ dependence is shown in Fig. 4. This quantity represents the limiting degree of ionization of a free atom with nuclear charge Z, when

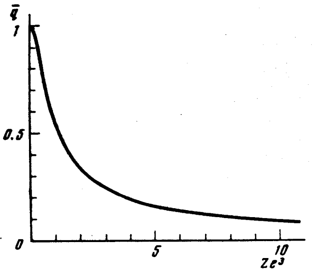

FIG. 4. Limiting degree of ionization of an atom with nuclear charge Z (radius of the nucleus $R = r_0 A^{1/3}$, $r_0 = 1.1$ F, $Z/A = 0.5$).

the outer electron shell is completely absent. An atom with nucleus Z and $q > q(Z)$ is unstable, and after spontaneous emission of several positrons, transforms into a stable ion with a filled vacuum shell (the degree of ionization decreases then to $\bar{q}(Z)$).

The relativistic Thomas-Fermi equation for the positive ion is solved by the method given in the previous section. Setting

$$V_q(r) = V(r) - V(r_0(q)), \tag{20}$$

where $Ze^3 \ll 1$, $0 \leq q \leq \bar{q}$, and $r_0(q)$ is the radius of the positive ion, we have the same equation (1) for $V_q(r)$ but with other boundary conditions:

$$V_q(r_0) = 0, \quad r_0^2 V_q'(r_0) = Ze^2 q. \tag{21}$$

The formula (14) is preserved for $V_q(r)$, and a_2 has its previous value, while the constant a_1 is expressed by Eq. (19), in which it is necessary to replace $\gamma \equiv \gamma(0)$ by $\gamma(q)$. The dependence of $\gamma(q) = -\chi'(0)$ on the degree of ionization q is well known from the nonrelativistic Thomas-Fermi model.[1,2] The value of $\gamma(q)$ also increases with increase in q.

At $Ze^3 \ll 1$, the division of the electron density $n_e(r)$ into two practically nonoverlapping parts (the vacuum and outer shells of the atom) is preserved also for the positive ions.

5. THE THOMAS-FERMI EQUATION AT SMALL DISTANCES. CALCULATION OF THE GELL-MANN–LOW FUNCTION IN ELECTRODYNAMICS WITH STRONG COUPLING ($Ze^3 \gg 1$)

"Falling to the center" arises in the Dirac equation with the potential $V(r) = -\zeta/r$ at $\zeta = 1$. To set up the problem correctly at $\zeta > 1$, we must introduce a cutoff of the Coulomb potential at small distances, which corresponds physically to account for the finite dimensions of the nucleus.[6] Let us consider how this phenomenon appears in the many-body problem of the electron shell of the supercritical atom.

At small distances from the nucleus, the contribution of the vacuum shell predominates in $n_e(r)$. If we denote its share in the electron density by ν, then

$$\nu(r) = \left\{\frac{|V(r)|-2}{|V(r)|+2}\right\}^{3/2} = 1 - \frac{6}{|V(r)|} + \ldots \quad \text{at} \quad |V(r)| \gg 1.$$

Therefore, it suffices to consider the case of the vacuum ion. Setting

$$\varphi(x) = -x(V+1), \quad x = r/r_0, \quad \mu = (Z_1 e^3)^2/3\pi, \tag{22}$$

we obtain the relativistic Thomas-Fermi equation in the form

$$x^2\varphi'' = \mu(\varphi^2 - x^2)^{3/2}, \quad r > R, \tag{23}$$

where

$$\varphi(1) = 1, \quad \varphi'(1) = -1. \tag{24}$$

It can be shown that the function $\varphi(x)$ increases monotonically with decrease in x and becomes infinite at some point $x = x_0(\mu)$ (see the Appendix). It follows from (23) that this singularity is a pole:

$$\varphi(x) = \frac{A}{x - x_0} + O(1), \quad x \to x_0; \qquad A = (2/\mu)^{1/2} x_0(\mu). \tag{25}$$

For the determination of the dependence of x_0 on the parameter μ, Eq. (23) has been solved numerically with the boundary conditions (24). The results are shown in Fig. 5, in which the continuous curve denotes the quantity $x_0(\mu)\exp(1/8\mu)$.

We now consider the properties of the solutions of Eq. (23) at small distances. The presence in (23) of the small parameter μ allows us to apply perturbation theory. Here it turns out that the real parameter of the expansion is not μ but $\mu \ln x$:

$$\varphi(x) = 2(1 - 4\mu \ln x + \ldots), \quad x \ll -\mu \ln x \ll 1 \tag{26}$$

(see the formula (A.7) in the Appendix). At $x \ll 1$, Eq. (1) simplifies to $x^2\varphi'' = \varphi^3$ and becomes invariant relative to the group of scale transformations:

$$\varphi \to \lambda^{1/2}\varphi, \quad \mu \to \lambda^{-1}\mu, \tag{27}$$

which leave the combination $\mu\varphi^2$ unchanged. It is convenient to transform to the variables $t = -\ln x$ and $\xi = \frac{1}{4}\mu\varphi^2$. The quantity ξ plays the role of an invariant charge:

$$V(r) = -\frac{Z_1 e^2}{r}\left[\frac{\xi(r,\mu)}{\mu}\right]^{1/2}. \tag{28}$$

We consider a region of r that is much greater than the distances $\sim \exp(-3\pi/2e^2)$ at which the problem of zero

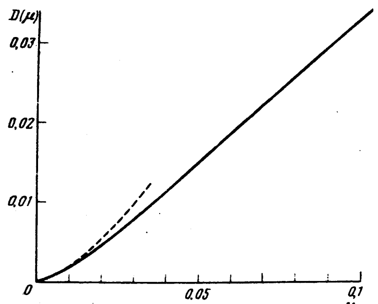

FIG. 5. Exponential cofactor $D(\mu) = x_0(\mu) \exp(1/8\mu)$ in Eq. (37); the continuous curve shows the results of numerical calculation, the dashed curve is the asymptote $D(\mu) = D\mu^{3/2}$.

charge in quantum electrodynamics arises.[10] For such r, we can neglect the vacuum polarization.[5,10] In the consideration of the effect of screening, it is sufficient to take into account the density of free charges present in the vacuum, $\rho(r) = -en_e(r)$, which is determined by the electrons of the vacuum shell.

For the invariant charge, we have the equation

$$\frac{\partial^2\xi}{\partial t^2}+\frac{\partial\xi}{\partial t}-\frac{1}{2\xi}\left(\frac{\partial\xi}{\partial t}\right)^2=8\xi^2. \tag{29}$$

The boundary condition for it is the solution (26) obtained from perturbation theory: $\xi(t, \mu) = \mu(1+8\mu t+\ldots)$. Since the coefficients in (29) do not depend on t, the solution has the form: $\xi(t, \mu) = F(t+\Phi(\mu))$. The normalization condition $\xi(0, \mu) = \mu$ gives the relation $F = \Phi^{-1}$, and we finally obtain

$$\Phi(\xi(t, \mu))=t+\Phi(\mu). \tag{30}$$

Thus, the solution of the relativistic Thomas-Fermi equation at small ($r \ll r_a$) distances has the form that is characteristic for the renormalized group,[14,15] and possesses the property of renormalizability.

For the Gell-Mann–Low function,

$$\beta(\mu)=\partial\xi(t, \mu)/\partial t|_{t=0}$$

we get from (29)

$$\beta'=-1+\beta/2\mu+8\mu^2/\beta; \qquad \beta=8\mu^2+\ldots, \quad \mu\to 0. \tag{31}$$

This equation is transformed to much simpler form if we transform to the variables g and $\psi(g)$:

$$g=2\mu^{1/2}, \quad \psi=\mu^{-1/2}\beta(\mu). \tag{32}$$

Here we get

$$\frac{d\psi}{dg}=-1+\frac{g^3}{\psi}; \quad \psi(g)=g^3+\ldots, \quad g\to 0. \tag{33}$$

As $g\to 0$, the functions $\psi(g)$ and $\beta(\mu)$ can be represented in the form of series of perturbation theory:

$$\psi(g)=g^3\sum_{k=0}^{\infty}a_k(-g^2)^k, \quad \beta(\mu)=\sum_{k=2}^{\infty}c_k(-\mu)^k, \tag{34}$$

where $c_k = 2^{2k-1}a_{k-2}$. As $k\to\infty$, the coefficients a_k and c_k increase factorially:

$$a_k\approx A(k!)2^k k^{1/2}[1+O(k^{-1})] \tag{35}$$

(see Eqs. (A.14), (A.15)). This shows that the series (34) have zero radius of convergence and are asymptotic. The Gell-Mann–Low function $\beta(\mu) = \mu^{1/2}\psi(2\mu)^{1/2}$ was found by numerical integration of Eq. (33). As is seen from Fig. 6, it is monotonically increasing and does not have positive zeros. We write out its asymptotic forms:

$$\beta(\mu)=\begin{cases}8\mu^2-96\mu^3+\ldots, & \mu\to 0\\ (2\mu)^{3/2}-\dfrac{2}{3}\mu+\ldots, & \mu\to\infty\end{cases} \tag{36}$$

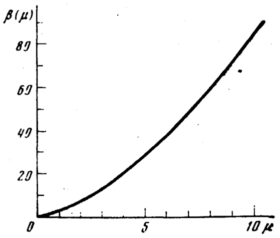

FIG. 6. The Gell-Mann–Low function for the problem of screening of the nuclear charge by the vacuum shell.

Thus, for the given example, the case of zero charge is realized.[15]

Using the above results, we can find the location of the pole $x_0(\mu)$ analytically in the solution of the problem (23) and (24) at small μ:

$$x_0(\mu)=D(\mu)e^{-1/8\mu}; \quad D(\mu)=D\mu^{3/4} \quad (\mu\to 0), \tag{37}$$

where $D\approx 1.86$ is a constant found by numerical integration (see Item 3 of the Appendix). We call attention to the nonanalytic character of $x_0(\mu)$ in the variable μ at the point $\mu = 0$. The asymptotic form of (37) is shown in Fig. 5 by the dashed line.

From the physical sense of the problem, the electron density $n_e(r)$ and the self-consistent potential $V(r)$ cannot become infinite. This leads to a condition on the radius of the nucleus R:

$$R>R_{cr}=\left(\frac{3\pi}{4e^2}\mu\right)^{1/2}x_0(\mu)=Cr_a(Z_1e^2)^2\exp\left(-\frac{3\pi}{8(Z_1e^2)^2}\right), \tag{38}$$

here C is a numerical factor. At fixed value of the outer charge Z_1, the radius of the nucleus R cannot be arbitrarily small—at $R<R_{cr}$, Eq. (1) does not have a bounded solution. This is how "falling to the center" manifests itself in the relativistic Thomas-Fermi equation.

We note that the dependence $\overline{Z}_1(R)$ shown in Fig. 2 is a function inverse to the function $R_{cr} = R_{cr}(Z_1)$.

The "critical" value of the radius R lies at exponentially small distances, exceeding by many orders of magnitude the characteristic radius $r_0 \sim \exp(-3\pi/2e^2)$ at which growth in the polarization of the vacuum takes place and the problem of zero charge arises in quantum electrodynamics[10,15] ($R_{cr}/r_0 \sim \exp\{3\pi(1-1/4\zeta^2)/2e^2\}$). At the same time, the value of R_{cr} is much smaller than the radii of superheavy nuclei ($R \gtrsim 0.03$); therefore, in the real problem of the vacuum shell of the supercritical atom, the pole $x_0(\mu)$ of the solution of Eq. (1) does not appear. However, account of the density of vacuum electrons as $r\to 0$ can be important in the consideration of the problem of zero charge in quantum electrodynamics.

6. FINAL REMARKS

1. The correct description of the vacuum shell of the supercritical nucleus was first given in Ref. 9 (in the single-particle approximation, i.e., the interaction $\propto Ze^2$ between electrons and the nucleus was taken into account exactly, and the interaction $\propto e^2$ between electrons and positrons was neglected). Similar results were subsequently obtained in Ref. 16. The numerical calcu-

lations[17] of the charge distribution of the vacuum shell, its mean radius, and other quantities confirm the conclusion of Ref. 9.

In these works, the case was considered of comparatively small Z (namely, $\zeta - \zeta_{cr} \ll \zeta_{cr} = 1.25$), when even fewer electrons are in the vacuum shell. In the present work, the inverse case $Z \gg Z_{cr}$ was investigated, when $N_e \gg 1$ and statistical description of the vacuum shell becomes possible.

2. At $Z > Z_{cr}$, it is impossible to neglect the interaction between the electrons. Equation (1) takes into account the Coulomb interaction between the electron shells. Since the electrons are relativistic, the question arises of account of retardation. It can be shown that the Breit terms in the interaction Hamiltonian $H_{int} = e^2(1 - \alpha_1 \alpha_2)/|\mathbf{r}_1 - \mathbf{r}_2|$, which are velocity dependent, vanish in summation over the closed subshell ($-j \leq M \leq j$) with fixed value of the angular momentum j. As is shown in Ref. 5, the exchange and correlation effects at $\zeta \gg 1$ give small corrections to Eq. (1). This serves as the basis for the applicability of the relativistic Thomas-Fermi equation to the static problem at $Ze^2 \gg 1$.

3. In recent years, A. B. Migdal and co-workers developed the theory of pion condensation[4] and showed that nuclear matter, beginning with some "critical" density n_c, becomes unstable to the creation of bound pions. As a consequence, a phase transition of the nucleus to a state with a pion condensate appears. The energy gain associated with the formation of the π condensate points to a possibility of the existence of anomalous nuclei with density several times the normal density n_0, and also of neutron ($N \gg Z$ and $Z \gtrsim 10^3$) and supercharged ($Ze^3 \gtrsim 1$) nuclei.[13] Theoretical calculations are very sensitive to the parameters of the NN- and πN-interactions in nuclear matter, which are not yet known with sufficient accuracy. The investigation of the properties of the electron shell of supercritical nuclei that we have carried out can turn out to be useful for the search for anomalous nuclei, which is very important at the present time (see, for example Refs. 19 and 20).

4. Equation (1) is based on the quasiclassical approximation, the condition of applicability of which to the Coulomb field at $Z > 137$ has the form $(\zeta^2 - 1)^{1/2} \gg 1$.[5,21] Actually, the region of applicability of the quasiclassical treatment extends to $(\zeta^3 - 1)^{1/2} \sim 1$ (thus, the error in the quasiclassical formulas for ζ_{cr} is[21] several percent even in the case of the 1s level, when $\zeta_{cr} = 1.25$; similarly, the total number of levels that are dropped to the lower continuum is well described[11] by Eq. (3) at $\zeta > 2$). This gives assurance that the distribution of the electron density in the shell of the supercritical atom can be obtained from the Thomas-Fermi equation with excellent accuracy, beginning with $\zeta = 1.5$–2. In Ref. 22, the values of the critical charge of the nucleus are calculated with the help of Eq. (1) for the excited levels ($2p_{1/2}$, $2s_{1/2}$, and so on) with account of the correction for screening of the Coulomb field of the nucleus by the vacuum shell.

5. We note an analogy between the properties of the relativistic Thomas-Fermi equation as $r \to 0$ and some equations of quantum field theory. In particular, the series (34) is similar to the series of perturbation theory for the Gell-Mann–Low function in scalar field theory with the interaction $H_{int} = g \int \varphi^4/4!\, d^4x$. According to Lipatov,[23] in this case,

$$\psi(g) = \sum_{k=2}^{\infty} c_k (-g)^k; \quad c_k = A(k!) a^k k^{7/2}, \quad k \to \infty, \tag{39}$$

where $A = (2\pi)^{-1/2} \tilde{C}(4) \approx 1.1$ and $a = (16\pi^2)^{-1}$. A comparison of Eqs. (39) and (35) shows that the asymptotic forms of the higher orders of perturbation theory in these two theories have identical structure and differ only in the values of the constants A and a. This analogy seems of interest to us and merits further study.

APPENDIX

We consider in more detail the properties of the solution of the relativistic Thomas-Fermi equation.

1. It is seen directly from (23) that $\varphi''(x) > 0$ at $x < 1$. With account of the boundary conditions (24), we have

$$\varphi'(x) = -\left(1 + \int_x^1 \varphi''(x)\, dx\right) < -1.$$

Therefore, $\varphi(x)$ is a monotonically decreasing function and $\varphi(x) > \varphi_0(x)$, where $\varphi_0(x) = 2 - x$ is the solution of the problem (23), (24) at $\mu = 0$. It then follows that the function $\varphi(x)/x$ increases without limit upon decrease in x and becomes infinite at some point $x = x_0(\mu)$.

2. We now find the location of the pole $x_0(\mu)$ explicitly in the case of weak coupling $\mu \to 0$ (i.e., $Ze^3 \ll 1$). Equation (23) at $x \ll 1$ takes the form

$$x^2 \varphi'' = \mu \varphi^3. \tag{A.1}$$

Since $\mu \to 0$, it is natural to solve this equation by perturbation theory:

$$\varphi(x, \mu) = \sum_{n=0}^{\infty} \mu^n \varphi_n(x). \tag{A.2}$$

After transition to the variable $t = -\ln x$, we obtain an equation with constant coefficients

$$d^2\varphi/dt^2 + d\varphi/dt = \mu \varphi^3, \tag{A.3}$$

which can be satisfied by the series (A.2) by setting

$$\varphi_n(x) = A_n t^n + B_n t^{n-1} + O(t^{n-2}), \quad t \to \infty. \tag{A.4}$$

Substituting this expansion in (A.3), we obtain the recurrence relations

$$A_n = \frac{1}{n} \sum_{i+j+k=n-1} A_i A_j A_k, \quad B_n = -nA_n + \frac{3}{n-1} \sum_{i+j+k=n-1} A_i A_j B_k.$$

The initial coefficients A_0 and B_1 are determined from expansions of the functions $\varphi_0(x)/x$ and $\varphi_1(x)/x$ obtained in Ref. 5:

$$A_0 = 2, \; B_0 = 0, \; B_1 = 8(2 \ln 2 - {}^{11}/_3).$$

The chain of equations for A_n is easily solved in general form:

$$A_n=2^{n+1}(2n)!(n!)^{-2}. \quad \text{(A.5)}$$

The equations for B_n are more cumbersome; however, we can determine the asymptotic coefficients for large n. In this case,

$$A_n\approx 2^{3n+1}(\pi n)^{-1/2}, \quad B_n\approx -2^{3n}\cdot 3(n/\pi)^{1/2}\ln n. \quad \text{(A.6)}$$

Summation of the leading terms of the expansion (A.2) gives

$$\varphi(x,\ \mu)=2(1-\tau)^{-1/2}+12\mu(1-\tau)^{-3/2}\ln(1-\tau)+\ldots, \quad \text{(A.7)}$$

where $\tau=-8\mu\ln x$. This function has a singularity at $\tau=1$, i.e., at $x=\exp(-1/8\mu)$.

Thus, an exponential dependence of $x_0(\mu)$ on the coupling constant μ is obtained in the case $\mu\to 0$. A comparison with (25) and (37), however, shows that the method of summation of the leading logarithmic terms does not give the correct form of the singularity of $\varphi(x)$ as $x\to x_c$ (and also the correct factors of the exponential in the expression for $x_0(\mu)$). The reason for this is made clear from the expansion (A.7): the correction terms, $\sim B_n t^{n-1}$, and also $\varphi_n(x)$ lead to a second term in (A.7), which contains an extra power of the small parameter μ, but, on the other hand, a more singular function as $\tau\to 1$. It is clear from this example that the solution near the singularity has nothing in common with the result of summation of the leading logarithmic terms. This is instructive, in view of the fact that the method of summation of the leading terms of the perturbation theory series is frequently employed in quantum field theory (see, for example, Ref. 10).

The expression (A.7) is valid in the region $\tau\ll 1$, where it gives the formula (26).

3. The exact asymptotic form of $x_0(\mu)$ as $\mu\to 0$ is conveniently obtained by using the property of the renormalizability of the solution of Eq. (A.1) at small distances:

$$\ln\frac{x}{x_0}=t_0-t=\int\limits_{\xi(t,\mu)}^{\infty}\frac{d\mu'}{\beta(\mu')}. \quad \text{(A.8)}$$

Substituting the expansion (36) for the Gell-Mann–Low function, we find

$$t_0-t=1/8\xi-{}^3/_2\ln\xi+b_0+b_1\xi+\ldots,$$
$$b_0=-\frac{1}{8}+\int\limits_0^1\left(\frac{1}{\beta(\mu)}-\frac{1}{8\mu^2}-\frac{3}{2\mu}\right)d\mu+\int\limits_1^{\infty}\frac{d\mu}{\beta(\mu)}. \quad \text{(A.9)}$$

The general form of the solution of Eq. (29) is obtained in this way in the region of application of perturbation theory ($\xi\ll 1$). On the other hand, for the vacuum shell we have $\xi(t,\mu)=\mu(1+8\mu(t+\ln 2-11/3)+\ldots)$, see Sec. 4 in Ref. 5. Substituting this expression in (A.9), we get Eq. (37) for $x_0(\mu)$, and the constant in the pre-exponential factor is equal to $D=\exp(-b_0+2\ln 2-11/3)=1.86\ldots$.

4. In the opposite case of large μ we have $x_0(\mu)\to 1$, so that Eq. (23) can be simplified:

$$\varphi''=\mu(\varphi^2-1)^{3/2}. \quad \text{(A.10)}$$

This equation is easily integrated in quadratures; the pole $x_0(\mu)$ corresponds to $\varphi=\infty$, whence

$$x_0(\mu)=1-\int\limits_1^{\infty}d\varphi\left[1+2\mu\int\limits_1^{\varphi}dy(y^2-1)^{3/2}\right]^{-1/2}. \quad \text{(A.11)}$$

In the integral over φ, the principal contribution is made by the region near $\varphi=1$, where

$$\int\limits_1^{\varphi}dy(y^2-1)^{3/2}=\frac{2^{7/2}}{5}(\varphi-1)^{5/2}+O((\varphi-1)^{7/2}).$$

Substituting this expression in (A.11) and calculating the integral over φ, we find

$$x_0(\mu)=1-b\mu^{-2/5}+\ldots,\quad \mu\to\infty, \quad \text{(A.12)}$$

where $b=2^{-2/5}5^{-3/5}B(2/5,1/10)=3.435$ (this asymptotic form is achieved only at very large values of μ).

5. For the calculation of the coefficients of the perturbation theory series, we start out from Eq. (33), which we rewrite in the form $\varphi\varphi'=g^3-\varphi$. Substituting the expansion (34) here, we obtain the recurrence relations

$$a_{k+1}=(k+3)\sum_{i+j=k}a_i a_j,\quad a_0=1, \quad \text{(A.13)}$$

whence $a_1=3$, $a_2=24$, $a_3=285$, $a_4=4284$, $a_5=75978,\ldots$. These coefficients increase rapidly. We seek the asymptotic value of a_k as $k\to\infty$ in the form

$$a_k\approx A\Gamma(k\alpha+1)a^k k^\beta. \quad \text{(A.14)}$$

Substituting this expression in (A.13), and recognizing that the principal contribution to the sum $\sum a_i a_j$ is made by terms with the maximum value of $|i-j|$, we find the parameters α, a, and β. It is not possible to find the constant A by this method. It was calculated from a comparison of the asymptotic form (A.14), with accurate values of the coefficients a_k calculated on a high speed computer from the recurrence relations (A.13) up to $k=200$. The final result is

$$\alpha=1,\ a=2,\ \beta={}^7/_2,\ A=0.04551\ldots \quad \text{(A.15)}$$

The asymptotic coefficients c_k of the Gell-Mann–Low function $\beta(\mu)$ have the same form as (A.14) except for the values of the parameters A, a, and β.

[1)] At $Ze^2>1$, the point-charge approximation is inapplicable,[6–9] and it is necessary to take into account the finite dimensions of the nucleus. As will be shown below (see Sec. 5), Eq. (1) does not have bounded solutions in the limit as $R\to 0$, where R is the radius of the nucleus.

[2)] The quantity Z_{cr} depends on the quantum numbers n and $\varkappa$. The sign of $\varkappa$, together with the energy ε, the angular momentum j, and its projections, is an integral of the motion in an arbitrary central field.[10] The values of Z_{cr} for the first levels of the discrete spectrum were calculated in Refs. 7 and 8: $Z_{cr}=169$, 181, 232 and 255 for the levels is $1s_{1/2}$, $2p_{1/2}$, $2s_{1/2}$, $3p_{1/2}$ (at $r_0=1.1$ F, and $A=2.6$ Z). A numerical calculation of Z_{cr} for a large number of states of the discrete spectrum has appeared recently.[11]

3) The function $f(r/R)$, which cuts off the growth of $V(r)$ at $r<R$, is determined by the distribution of protons inside the nucleus. The following models of cutoff are used most frequently: I) $f(x)=1$ at $0<x<1$; II) $f(x)=(3-x^2)/2$, which corresponds to constant density of protons of form (3). According to the terminology used in Refs. 8, 9, and 11, these models are known as model I and model II, respectively.

4) The idea of the possibility of formation of a π-condensate in nuclei was expressed in Ref. 12. Detailed references to subsequent works and a discussion of the present status of the theory of the π-condensate can be found in Ref. 18.

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Parity nonconservation effects in two-photon transitions in hydrogen atoms

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Parity nonconservation effects in two-photon transitions $1s_{(1/2)}\to 2p_{(1/2)}$ and $2s_{(1/2)}\to 2p_{(3/2)}$ in a hydrogen atom arising if the neutral weak currents do not conserve parity are considered. The magnitude of the effects in the general case is 10^{-8}–10^{-9}. However, in the case of absorption of photons with equal energies and parallel or antiparallel momenta in the transition $1s_{(1/2)}\to 2p_{(1/2)}$ the magnitude of these effects increases and attains values of 10^{-4}–10^{-6}.

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The discovery in 1973 of weak neutral currents[1,2] opened up new possibilities for the study of weak interaction by means of looking for the effects brought about by this interaction of nonconservation of parity in atomic transitions. One can expect particularly large effects in transitions which in the absence of weak interactions are for some reason suppressed. There is available a large number of theoretical papers in which the effect of weak interaction on one-photon transitions in atoms is discussed (cf., the review articles[3,4]).

Also of interest are effects of parity nonconservation in two-photon atomic transitions. Experiments on induced two-photon transitions in an atom have received wide application recently due to progress in laser technology. The study of such transitions occurring as a result of a simultaneous absorption of two photons whose total energy is equal to the energy of the transition has a number of advantages compared to the study of the usual one-photon transitions. Among them are, for example, the extension of the range of energies of transitions

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