

Coulomb problem for a $Z > Z_{\text{cr}}$ nucleus

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Abstract. A closed-form equation is derived for the critical nucleus charge $Z = Z_{\text{cr}}$ at which a discrete level with the Dirac quantum number touches the lower continuum of the Dirac equation solutions. For the Coulomb potential cut off rectangularly at the short distance $r_0 = R\hbar/mc$, $R \ll 1$, the critical nucleus charge values are obtained for several values of κ and R . It is shown that the partial scattering matrix of elastic positron–nucleus scattering, $S_\kappa = \exp(2i\delta_\kappa(\varepsilon_p))$, is also unitary for $Z > Z_{\text{cr}}$. For this range, the scattering phase $\delta_\kappa(\varepsilon_p)$ is calculated as a function of the positron energy $E_p = \varepsilon_p mc^2$, as are the positions and widths of quasidecrete levels corresponding to the scattering matrix poles. The implication is that the single-particle approximation for the Dirac equation is valid not only for $Z < Z_{\text{cr}}$ but also for $Z > Z_{\text{cr}}$ and that there is no spontaneous creation of e^+e^- pairs from the vacuum.

Keywords: Coulomb problem, point-like nucleus, boundary conditions, critical charge, scattering phase, Breit–Wigner resonance

1. Introduction

The following formula for the discrete level energies ε_d in the relativistic Coulomb problem was obtained by Sommerfeld [1] using Bohr’s theory of the atom long before Dirac derived his famous equation for the electron; it was then rederived by applying the Dirac equation to the field of a

point-like charge Z (in electron charge units) [2–5] (see also the monographs [6, 7]):

$$\varepsilon_{n_r}(\kappa; Z) = \left[1 + \frac{(Z\alpha)^2}{\left(\sqrt{\kappa^2 - (Z\alpha)^2} + n_r\right)^2} \right]^{-1/2}, \quad (1)$$

$$n_r = \begin{cases} 0, 1, 2, \dots, & \kappa < 0, \\ 1, 2, \dots, & \kappa > 0. \end{cases}$$

Here, the Dirac quantum number $\kappa = \mp(j + 1/2)$ is an eigenvalue of the operator $K = \beta(1 + \Sigma \mathbf{L})$ [8, 9], j is the conserved total angular momentum of the electron, and n_r is the analog of the radial quantum number in the Schrödinger theory. The system of units most commonly used is one in which $\hbar = c = m = 1$, with the fine structure constant $\alpha = e^2/(\hbar c) \simeq 1/137.04$ (where m and $-e$ are the electron mass and charge).

For the ground state ($1s_{1/2}$: $\kappa = -1$, $n_r = 0$), energy (1) vanishes at $Z = 137$, whereas for $Z > 137$ it becomes complex-valued, making the Sommerfeld formula meaningless. However, as noted by Pomeranchuk and Smorodinsky [10], this is true only for a point-like charge. For finite radius nuclei, the energy of the lowest discrete level increases with Z until it reaches the boundary of the lower continuum of the Dirac equation solutions at a certain ‘critical’ charge $Z = Z_{\text{cr}}$. Calculating Z_{cr} for a rectangularly cut-off Coulomb potential (surface charge distribution) for the nuclear radius $r_0 = 12 \text{ F}$ (which corresponds to $R = 0.031$ in units of $\hbar/(mc) = 3.86 \times 10^{-11} \text{ cm}$) yielded the overestimated value $Z_{\text{cr}} = 200$ in [10]. An exact bare-nucleus calculation with the same model yields $Z_{\text{cr}} = 177$ [11, 12].

If Z becomes larger than Z_{cr} , the first discrete level disappears from the spectrum. There is an analogy between this ground level behavior in the Coulomb problem and the way the levels in a rectangular potential well move as the well depth increases. It was shown by Schiff, Snyder, and Weinberg [13] that for a certain depth V_0 , the lowest-energy level goes down to $-mc^2$. As the well is deepened further, this level disappears, moving into the (lower) continuum spectrum. In [10], this is explained based on the interpretation by Schiff, Snyder, and Weinberg by suggesting that if we place an electron in the field of a supercritical nucleus, the electron

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disappears and the vacuum charge decreases by one electron charge, which means that the electron collapses onto the nucleus.

According to later work (see papers [11, 12, 14–23] and monographs [8, 24, 25]), a bare $Z > Z_{\text{cr}}$ nucleus allows e^+e^- pair production from the vacuum, with the positrons escaping to infinity and the electrons remaining to screen the nucleus charge, which decreases by two units and forms a supercritical atom [23]. We show in what follows that this interpretation of what occurs at $Z > Z_{\text{cr}}$ is invalid: once a discrete level has reached the boundary of the lower continuum, it disappears by colliding with a virtual level to combine with it into a pair of complex-energy Breit–Wigner levels on the second, nonphysical sheet. The level that is closer to the physical region and has the energy $\varepsilon_{\text{BW}}^{(+)} = -\varepsilon_0 + i\gamma/2$ with $\varepsilon_0 > 1$ and $\gamma > 0$ corresponds to the resonance in the scattering of positrons with the energy $\varepsilon_{\text{p}} = -\varepsilon \geq 1$ by the nucleus, the complex energies of the quasistationary state being $\varepsilon_{\text{qs}} = -\varepsilon_{\text{BW}}^{(+)} = \varepsilon_0 - i\gamma/2$, where ε_0 and γ are respectively the position and width of the quasidiscrete level.¹

In recent years, the subject under discussion has proved to be of topical interest to the physics of nonrelativistic two-dimensional structures, a field apparently remote from nuclear physics. The reason is that, depending on the substrate, the properties of graphene are described by an effective gapless or gapped two-dimensional Dirac equation (see, e.g., Refs [26–28]). In the presence of a Coulomb impurity, the energy spectrum of a two-dimensional Coulomb problem is determined (due to the axial symmetry) by a system of equations that, except for a difference in notation, is precisely the three-dimensional radial Dirac system considered in this paper. We note that the effective fine structure constant then turns out to be larger than $1/137$ and that Z_{cr} is close to unity [29]. This offers the unique possibility of experimentally testing the theory of supercritically charged atoms.

In Section 2, we discuss the boundary conditions that ensure that the radial Dirac Hamiltonian is self-adjoint. In Section 3, we briefly consider the short-range Coulomb problem in which the self-adjointness property is ensured by modifying the potential at short distances. In Section 4, we obtain the wave functions of the discrete levels and calculate both their energies and the corresponding critical charges. In Section 5, we consider the wave functions of the lower continuum and discuss the scattering matrix and its poles at complex energies corresponding to the positions and widths of quasistationary states for $Z > Z_{\text{cr}}$. Concluding remarks are in Section 6. The calculation of the critical charge Z_{cr} is briefly discussed in the Appendix.

2. Boundary conditions

The radial functions of the Dirac equation with the Coulomb potential $V_C(r) = -Z\alpha/r$ satisfy the system of equations [8]

$$H_D \Psi_{\varepsilon, \kappa}(r) = \varepsilon \Psi_{\varepsilon, \kappa}(r), \quad (2)$$

$$H_D = \begin{pmatrix} 1 - \frac{Z\alpha}{r} & \frac{d}{dr} - \frac{\kappa}{r} \\ -\frac{d}{dr} - \frac{\kappa}{r} & -1 - \frac{Z\alpha}{r} \end{pmatrix}, \quad \Psi_{\varepsilon, \kappa} = \begin{pmatrix} F(r) \\ G(r) \end{pmatrix},$$

where ε is the dimensionless energy, and the Dirac quantum number κ takes the values $\kappa = \pm 1, \pm 2, \dots$. It is known that because the Coulomb potential $V_C(r)$ ‘dies out’ at long distances, the parts of the spectrum that correspond to the ranges $\varepsilon \geq 1$, $-1 < \varepsilon_d < 1$, and $\varepsilon \leq -1$ are respectively the upper continuum of the Dirac equation solutions, the discrete spectrum, and the lower continuum [8].²

For the differential operator H_D to become an operator H acting in the Hilbert space $\mathcal{H} = \mathcal{L}^2(R_+)$ of square integrable functions on the real axis $R_+ = [0, \infty)$ with the Hermitian scalar product and norm defined by

$$(\Psi_2, \Psi_1) = \int_0^\infty \Psi_2^+(r) \Psi_1(r) dr \quad (3)$$

and

$$(\Psi, \Psi) = |\Psi|^2 = \int_0^\infty (|F(r)|^2 + |G(r)|^2) dr, \quad (4)$$

it is necessary that H_D satisfy certain boundary conditions. Because H is unbounded, the minimal necessary requirement on it is that it satisfy the conditions [30]

$$H\Psi = H_D\Psi, \quad D(H) = \{\Psi \in \mathcal{L}^2(R_+), H_D\Psi \in \mathcal{L}^2(R_+)\}, \quad (5)$$

where $D(H)$ is the domain of H . As a result, in accordance with (4), not only $F(r)$ and $G(r)$ but also their derivatives are square integrable. This can be seen by noting that the second condition in (5) gives

$$(H_D\Psi, H_D\Psi) = \int_0^\infty \left(|F+G|^2 + \left| \frac{d}{dr} F \right|^2 + \left| \frac{d}{dr} G \right|^2 \right) dr < \infty,$$

where the first term in the right-hand side is clearly convergent due to the triangle inequality $|F+G|^2 \leq |F|^2 + |G|^2$ and the first condition in (5). We finally have

$$\int_0^\infty |F|^2 dr < \infty, \quad \int_0^\infty \left| \frac{dF}{dr} \right|^2 dr < \infty, \\ \int_0^\infty |G|^2 dr < \infty, \quad \int_0^\infty \left| \frac{dG}{dr} \right|^2 dr < \infty,$$

and hence (see, e.g., Ref. [30]),

$$F(\infty) = G(\infty) = 0. \quad (6)$$

Integrating here by parts, we obtain

$$\int_0^\infty \Psi_2^+(H_D\Psi_1) dr - \int_0^\infty (H_D\Psi_2)^+ \Psi_1 dr \\ = \lim_{r \rightarrow 0} (F_1(r)G_1^*(r) - F_2^*(r)G_2(r)). \quad (7)$$

Thus, to ensure the self-adjointness property of the Hamiltonian, i.e., to reduce the boundary term to zero, it is essential to consider how the solutions of system (2) behave at short distances. This asymptotic behavior is determined by

¹ In [11, 12, 14–25], the width γ of the Breit–Wigner level is interpreted as the probability of spontaneous e^+e^- pair production from the vacuum.

² For $Z = Z_{\text{cr}}$, the $\varepsilon_d = -1$ state belongs to the discrete spectrum, and the $\varepsilon < -1$ states form the lower continuum.

the value of a single parameter, $\sigma = \sqrt{\kappa^2 - (Z\alpha)^2}$,³

$$\Psi_{\varepsilon, \kappa}(r \rightarrow 0) = C_\sigma \left\{ \eta_\sigma r^\sigma \left(\frac{1}{\sigma - \kappa} \frac{Z\alpha}{\sigma - \kappa} \right) + \eta_{-\sigma} r^{-\sigma} \left(\frac{1}{-\sigma - \kappa} \frac{Z\alpha}{-\sigma - \kappa} \right) \right\}, \quad (8)$$

$$\sigma \neq \frac{1}{2}, 0.$$

If $\sigma \geq 1/2$, then the square integrability of solutions in Eqn. (8) is achieved by setting $\eta_{-\sigma} = 0$. Therefore, the inequality $Z\alpha < \sqrt{\kappa^2 - 1/4}$ enables satisfying the so-called built-in boundary condition [30], and the Sommerfeld formula is valid for the energy levels. In particular, for the ground state with $\kappa = -1$, this leads to the inequality $Z < \sqrt{3}/2\alpha \approx 119$.

For $0 < \sigma < 1/2$, in accordance with von Neumann's theory of unbounded operators [31] (see also [32]), we require the boundary term in Eqn (7) to vanish due to the functions Ψ_1 and Ψ_2 that enter this equation on equal footing, and thus arrive at the condition

$$\frac{\eta_\sigma}{\eta_{-\sigma}} = \left(\frac{\eta_\sigma}{\eta_{-\sigma}} \right)^* = \tan \theta_\sigma(\kappa), \quad (9)$$

$$-\frac{\pi}{2} \leq \theta_\sigma(\kappa) \leq \frac{\pi}{2}, \quad \sigma = \sqrt{\kappa^2 - (Z\alpha)^2} > 0.$$

Condition (9) defines a one-parameter family of self-adjoint operators $H_{\theta_\sigma}^+ = H_{\theta_\sigma}$. We note that for the parameter values $\theta_\sigma = \pm\pi/2$, the Sommerfeld formula remains valid for Z up to $Z = |\kappa|/\alpha$, i.e., up to $Z < 137$ for the ground state.

If $Z\alpha > |\kappa|$, then, instead of Eqn (9), we obtain

$$\frac{\eta_\tau}{\eta_{-\tau}} = \left(\frac{\eta_\tau}{\eta_{-\tau}} \right)^* = \exp(2i\theta_\tau(\kappa)), \quad (10)$$

$$\text{Im } \theta_\tau(\kappa) = 0, \quad \tau = \sqrt{(Z\alpha)^2 - \kappa^2} > 0.$$

Boundary conditions (9) and (10) determine one-parameter families of self-adjoint radial operators H_{θ_σ} and H_{θ_τ} . For an alternative derivation of these one-parameter families, we refer the reader to Ref. [9].

3. Short-range Coulomb problem

To fix the parameters $\theta_\sigma(\kappa)$ and $\theta_\tau(\kappa)$, additional physical considerations are needed. According to Pomeranchuk and Smorodinsky, we should consider a Coulomb potential modified at short distances. For a rectangular cutoff [10]

$$V_R(r) = -\frac{Z\alpha}{R}, \quad r < R, \quad (11)$$

$$V_R(r) = -\frac{Z\alpha}{r}, \quad r > R, \quad R \ll 1,$$

system (2) with the replacement $V_C(r) \rightarrow V_R(r)$ can be solved at $r < R$ analytically in terms of the Bessel function. For $r < R$, i.e., at short distances,

$$\Psi_\kappa(r) = C_\kappa \sqrt{Z\alpha} \frac{r}{R} \left(\begin{matrix} \pm J_{\mp(1/2+\kappa)} \left(Z\alpha \frac{r}{R} \right) \\ J_{\pm(1/2-\kappa)} \left(Z\alpha \frac{r}{R} \right) \end{matrix} \right), \quad r \leq R \ll 1, \quad (12)$$

³ For $\sigma = 1/2, 0$, logarithmic ($\ln r$) terms arise in asymptotic form (8).

with the upper (lower) signs corresponding to $\kappa < 0$ ($\kappa > 0$).

Requiring the continuity of wave functions (12), noting the asymptotic form (8) at $r = R$ for $Z\alpha < |\kappa|$, and using Eqn (9), we obtain

$$\tan \theta_\sigma(\kappa, R) = \frac{(\sigma - \kappa) [Z\alpha J_{\mp(1/2+\kappa)}(Z\alpha) \pm (\sigma + \kappa) J_{\pm(1/2-\kappa)}(Z\alpha)] R^{-\sigma}}{(\sigma + \kappa) [Z\alpha J_{\mp(1/2+\kappa)}(Z\alpha) \mp (\sigma - \kappa) J_{\pm(1/2-\kappa)}(Z\alpha)] R^\sigma}, \quad (13)$$

$$\sigma = \sqrt{\kappa^2 - (Z\alpha)^2} > 0,$$

where, as in Eqn (12), the upper (lower) signs correspond to negative (positive) values of κ .

If $Z\alpha > |\kappa|$, then, according to Eqn (10), we have the equality

$$\exp(2i\theta_\tau(\kappa, R)) = \frac{(i\tau - \kappa) [Z\alpha J_{\mp(1/2+\kappa)}(Z\alpha) \pm (i\tau + \kappa) J_{\pm(1/2-\kappa)}(Z\alpha)] R^{-i\tau}}{(i\tau + \kappa) [Z\alpha J_{\mp(1/2+\kappa)}(Z\alpha) \mp (i\tau - \kappa) J_{\pm(1/2-\kappa)}(Z\alpha)] R^{i\tau}}, \quad (14)$$

$$\tau = \sqrt{(Z\alpha)^2 - \kappa^2} > 0.$$

Boundary conditions (9) and (13), together with Eqns (10) and (14), determine the wave functions of both the continuous and discrete spectra of system (2) in model (11) for any Dirac quantum number κ and the nuclear charge Z (including $Z > Z_{cr}$).

4. Discrete spectrum

For $\sigma = \sqrt{\kappa^2 - (Z\alpha)^2} > 0$, setting $\rho = 2\lambda r$ and $\lambda = \sqrt{1 - \varepsilon^2} \geq 0$ and following Ref. [6], we obtain the solutions of Eqn (2) decaying at infinity in the form

$$\begin{pmatrix} F \\ G \end{pmatrix} = C \sqrt{1 \pm \varepsilon} \exp\left(-\frac{\rho}{2}\right) \rho^\sigma \times \left\{ \Psi(a, c; \rho) \pm \left(\kappa + \frac{Z\alpha}{\lambda} \right) \Psi(a + 1, c; \rho) \right\}, \quad (15)$$

where C is the normalization factor, $\Psi(a, c; \rho)$ is the two-parameter Tricomi function ($a = \sigma - Z\alpha\varepsilon/\lambda$ and $c = 1 + 2\sigma$) [33], and the upper (lower) sign refers to the function $F(G)$.

With Eqn (9), we then obtain the equation

$$\frac{(2\lambda)^\sigma [Z\alpha\sqrt{1 - \varepsilon} + (\kappa - \sigma)\sqrt{1 + \varepsilon}] \Gamma(1 + \sigma - Z\alpha\varepsilon/\lambda) \Gamma(-2\sigma)}{(2\lambda)^{-\sigma} [Z\alpha\sqrt{1 - \varepsilon} + (\kappa + \sigma)\sqrt{1 + \varepsilon}] \Gamma(1 - \sigma - Z\alpha\varepsilon/\lambda) \Gamma(2\sigma)} = \tan \theta_\sigma(\kappa), \quad -\frac{\pi}{2} \leq \theta_\sigma(\kappa) \leq \frac{\pi}{2}, \quad (16)$$

which, together with equality (13), determines the discrete spectrum for $Z\alpha < |\kappa|$ in model (11).

If $Z\alpha > |\kappa|$, then, with $\tau = [(Z\alpha)^2 - \kappa^2]^{1/2} > 0$, we have the equation

$$\frac{(2\lambda)^{i\tau} [Z\alpha\sqrt{1 - \varepsilon} + (\kappa - i\tau)\sqrt{1 + \varepsilon}] \Gamma(1 + i\tau - Z\alpha\varepsilon/\lambda) \Gamma(-2i\tau)}{(2\lambda)^{-i\tau} [Z\alpha\sqrt{1 - \varepsilon} + (\kappa + i\tau)\sqrt{1 + \varepsilon}] \Gamma(1 - i\tau - Z\alpha\varepsilon/\lambda) \Gamma(2i\tau)} = \exp(2i\theta_\tau(\kappa)), \quad \text{Im } \theta_\tau(\kappa) = 0, \quad (17)$$

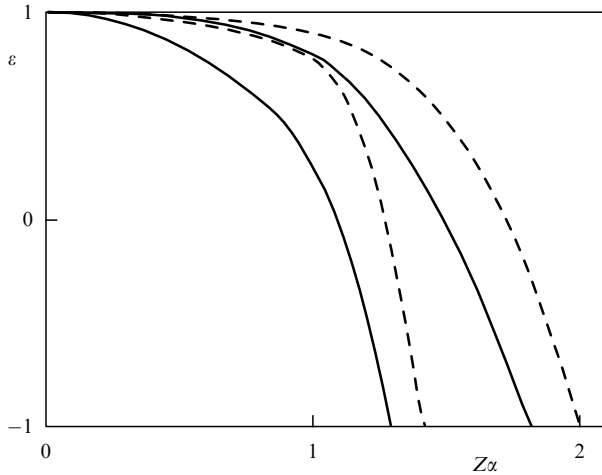


Figure 1. Energies of the ground state and the first excited state, $\varepsilon(Z\alpha, \kappa; R)$, versus the charge $Z\alpha$ for the Coulomb potential cutoff radius $R = 0.031$ (nucleus radius $r_0 = 12$ F) for $\kappa = -1$ (solid lines) and $\kappa = 1$ (dashed lines).

which, together with equality (14), determines the energy spectrum for $Z\alpha > |\kappa|$ in the same model.

Setting $\varepsilon = -1$ in Eqn (17) and noting the large-argument asymptotic behavior of the gamma function $\Gamma(1 \pm i\tau - Z\alpha\varepsilon/\lambda)$ yields the following equation for the critical charge $Z_{\text{cr}}^{(n)}(\kappa)$ at which the n th level with a given quantum number κ reaches the boundary of the lower continuum:

$$\arg \Gamma \left[2i \sqrt{(Z_{\text{cr}}^{(n)} \alpha)^2 - \kappa^2} \right] = \sqrt{(Z_{\text{cr}}^{(n)} \alpha)^2 - \kappa^2} \ln (2Z_{\text{cr}}^{(n)} \alpha) - \theta_{\tau}(\kappa) + \pi n, \quad (18)$$

where $n = 0, 1, 2, \dots$. Equation (18) combined with equality (14) determines the critical charge $Z_{\text{cr}}^{(n)}(\kappa, R)$ as a function of the quantum numbers κ and n and the cutoff radius R . Figure 1 shows the energies of the ground state and excited levels for $\kappa = -1$ and $\kappa = 1$ as functions of the charge in the range $0 < Z \leq Z_{\text{cr}}$ for $R = 0.031$. The accuracy of approximate Eqn (18) as a function of the cutoff radius is shown in Table 1.

5. Lower continuum wave functions

Noting the second linearly independent solution of the degenerate hypergeometric equation and setting $k = \sqrt{\varepsilon^2 - 1}$, we obtain the wave functions of the lower continuum solutions of system (2) in the form

$$\begin{aligned} \begin{pmatrix} F \\ iG \end{pmatrix} &= \exp \left(\mp i \frac{\pi}{2} \right) \sqrt{-\varepsilon \mp 1} (-2ikr)^{i\tau} \left\{ A \exp(ikr) \right. \\ &\times \left[\Psi(g_-, h; -2ikr) \pm \left(\kappa + i \frac{Z\alpha}{k} \right) \Psi(g_- + 1, h; -2ikr) \right] \\ &\pm B \exp(-ikr) \\ &\left. \times \left[\Psi(g_+, h; 2ikr) \pm \left(\kappa - i \frac{Z\alpha}{k} \right) \Psi(g_+ + 1, h; 2ikr) \right] \right\}. \quad (19) \end{aligned}$$

Here $g_{\pm} = i\tau \pm iZ\alpha\varepsilon/k$, $h = 1 + 2i\tau$, $\tau = [(Z\alpha)^2 - \kappa^2]^{1/2}$, $Z > Z_{\text{cr}}$, and the upper (lower) sign refers to the function F (iG).

Table 1. Critical charge $Z_{\text{cr}}^{(n)}(\kappa, R)$ in the rectangular cutoff model for the nucleus radius $r_0 = Rh/(mc)$ (1) calculated numerically in Ref. [11] (see the Appendix) and (2) calculated from approximate equation (18) using equality (14).

r_0, F	$1s_{1/2}$	$2p_{1/2}$	$2s_{1/2}$	Method
8	171	185	236	1
	172	187	236	2
10	174	189	244	1
	175	192	243	2
12	177	193	251	1
	178	196	249	2

Comparing these expressions with asymptotic form (8) with $\sigma = i\tau$ yields

$$\begin{aligned} u_{\tau} &= \Gamma(-2i\tau)(2k)^{i\tau}(Aa - Bb), \\ u_{-\tau} &= \Gamma(2i\tau)(2k)^{-i\tau}[A \exp(-\pi\tau)b^* - B \exp(\pi\tau)a^*], \end{aligned} \quad (20)$$

where

$$\begin{aligned} a &= \frac{Z\alpha\sqrt{-\varepsilon+1} - (i\kappa + \tau)\sqrt{-\varepsilon-1}}{\Gamma(1 - i\tau - i(\varepsilon/k)Z\alpha)}, \\ b &= \frac{Z\alpha\sqrt{-\varepsilon+1} + (i\kappa + \tau)\sqrt{-\varepsilon-1}}{\Gamma(1 - i\tau + i(\varepsilon/k)Z\alpha)}. \end{aligned} \quad (21)$$

Hence, with boundary condition (10), it follows that

$$\begin{aligned} \exp(-\pi\tau) \frac{B}{A} &= \exp(2i\delta_{\kappa}(k; Z)) = \frac{f_{\kappa}^*(k; Z)}{f_{\kappa}(k; Z)}, \\ A &= \frac{\exp(i\delta_{\kappa})}{\sqrt{2\pi(-\varepsilon)}} \exp\left(\frac{\pi Z\alpha(-\varepsilon)}{2k}\right), \end{aligned} \quad (22)$$

where $\delta_{\kappa}(k; Z)$ is the scattering phase,

$$f_{\kappa}(k; Z) = -i \left[\exp\left(\frac{\pi\tau}{2} - i\varphi_{\tau}\right) a - \exp\left(\frac{-\pi\tau}{2} + i\varphi_{\tau}\right) b^* \right] \quad (23)$$

is the Jost function, the constant factor A is determined from the normalization of the wave function to $\delta(k - k')$, and we have introduced the notation

$$\exp(i\varphi_{\tau}) = \frac{(2k)^{-i\tau} \Gamma(2i\tau)}{(2k)^{i\tau} \Gamma(-2i\tau)} \exp(2i\theta_{\tau}(\kappa)). \quad (24)$$

The scattering phase $\delta_{\kappa}(k; Z)$ for $\kappa = -1$ as a function of $Z = 232 > Z_{\text{cr}}$ is shown in Fig. 2, which should be compared with Fig. 13.3(a) in Ref. [34] for nonrelativistic resonance scattering, in which the background phase shift is zero, the phase δ jumps from 0 to π , and the cross section for $\delta = \pi/2$ reaches the unitary limit. The dashed-dotted line shows the asymptotic form of the phase at small positron momenta,

$$\delta_{\kappa}(k; Z) = \frac{Z\alpha}{k} \ln\left(\frac{Z\alpha}{ek}\right) + \frac{\pi}{4}. \quad (25)$$

The Gamow wave functions of quasistationary states follow from functions (19) by setting $B = 0$. This condition leads to the following equation for the complex energy spectrum of the quasidecrete levels corresponding

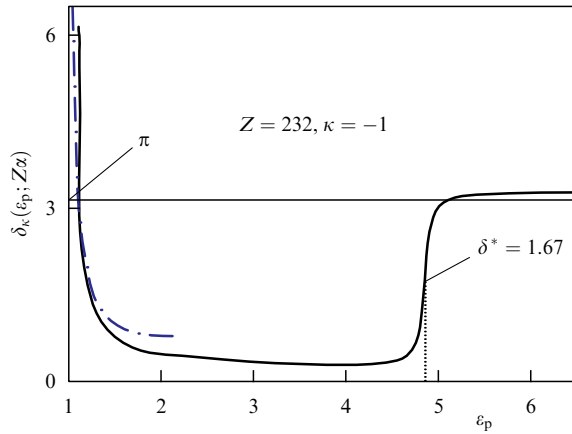


Figure 2. Scattering phase $\delta_\kappa(\epsilon_p; Z\alpha)$ for $\kappa = -1$ versus the positron energy for $Z = 232$ in the interval $Z_{cr}^{(0)}(-1, R) = 177 < 251 = Z_{cr}^{(1)}(-1, R)$ for $R = 0.031$ (solid line). The dashed-dotted line is the asymptotic phase for small positron momenta, Eqn (25), and δ^* is the phase corresponding to the positron energy ϵ^* .

to poles of the partial scattering matrix $S_\kappa(k; Z) = \exp(2i\delta_\kappa(k; Z))$:

$$\frac{(-2ik)^{i\tau} [Z\alpha\sqrt{-\epsilon+1} - (\tau+i\kappa)\sqrt{-\epsilon-1}] \Gamma(1+i\tau-iZ\alpha\epsilon/k) \Gamma(-2i\tau)}{(-2ik)^{-i\tau} [Z\alpha\sqrt{-\epsilon+1} + (\tau-i\kappa)\sqrt{-\epsilon-1}] \Gamma(1-i\tau-iZ\alpha\epsilon/k) \Gamma(2i\tau)} = \exp(2i\theta_\tau(\kappa)). \quad (26)$$

The solution of Eqn (26) determines both the position ϵ_0 and the width γ of a quasidiscrete level,

$$\epsilon = -\epsilon_0 + \frac{i}{2}\gamma, \quad \epsilon_0 > 0, \quad \gamma > 0, \quad (27)$$

and we note that for $\gamma \ll \epsilon_0$,

$$k_0 = k'_0 - ik''_0, \quad k'_0 = \sqrt{\epsilon_0^2 - 1}, \quad k''_0 = \gamma \frac{\epsilon_0}{2k'_0} > 0. \quad (28)$$

We note that the unusual sign⁴ in front of the quasistationary state width γ ensures that a discrete level for $Z > Z_{cr}$ moves to the nonphysical sheet, thereby ensuring the consistency of the one-particle approximation [35, 36] for the Dirac equation applied to the current problem, whereas the Klein–Fock–Gordon equation leads to contradictions.

The trajectories traced out, as Z increases, by the S -matrix poles in the plane of the complex variable $k = \sqrt{\epsilon^2 - 1} = k'_0 - ik''_0$ near the lower continuum boundary⁵ (Fig. 3) can be compared with the trajectories (see Fig. 13.6(a) in Ref. [34]) of the poles of the nonrelativistic elastic scattering amplitude of slow particles with a nonzero orbital momentum, when a centrifugal rather than a Coulomb barrier determines the presence of a resonance.

For $Z < Z_{cr}(\kappa)$, the energy of a discrete level is in the range $-1 < \epsilon_d < 1$, and hence $k_d = i\lambda_d$, $\lambda_d > 0$, and the

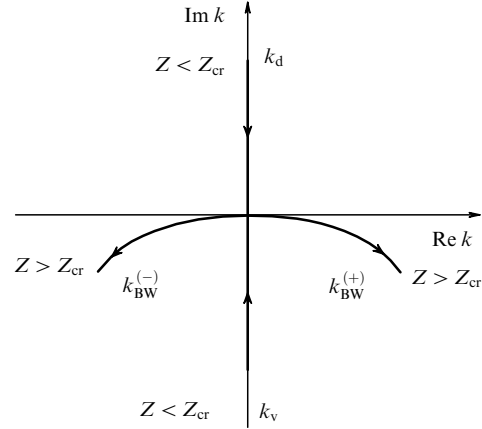


Figure 3. Trajectories of the S -matrix poles in the complex plane $k = \sqrt{\epsilon^2 - 1}$ close to the boundary of the lower continuum $\epsilon = -1$. The arrows indicate the direction of the trajectory as the charge Z increases.

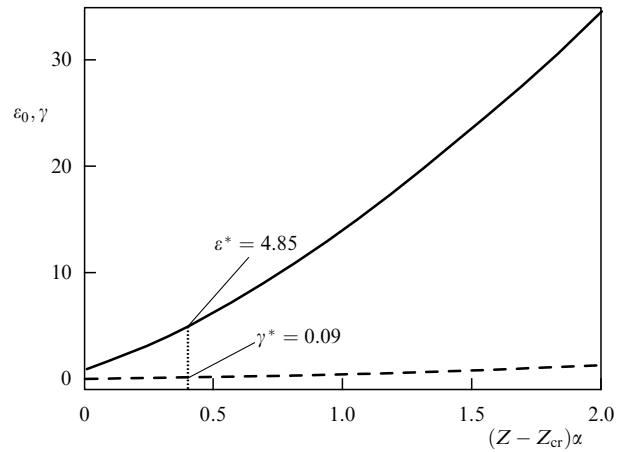


Figure 4. Resonance position $\epsilon_0(Z\alpha; \kappa = -1; R)$ (solid line) and the resonance width $\gamma(Z\alpha; \kappa = -1; R)$ (dashed line) versus the difference $(Z - Z_{cr})\alpha$ for the Coulomb potential cutoff radius $R = 0.031$. ϵ^* and γ^* are the position and width of the S -matrix pole that correspond to the resonance at $Z = 232$.

corresponding scattering matrix pole resides on the imaginary axis of the upper k -half-plane, i.e., on the first physical sheet. As the charge increases, this level approaches the lower continuum boundary $\epsilon = -1$; in the lower half-plane of complex k , moving opposite to it, also along the imaginary axis, there is a virtual level k_v that resides on the second, unphysical sheet. At $Z = Z_{cr}(\kappa)$, these levels collide, and as Z increases further, they become a pair of Breit–Wigner poles on the unphysical sheet. We note that in the supercritical region, the pole $k_{BW}^{(+)}$ that is closest to the positive real half-axis and which corresponds to quasistationary state (27) manifests itself as a resonance of the width γ in positron scattering by a supercritical charge.

Figure 4 shows how the position $\epsilon_0(Z, R)$ of the ‘ground’ (for $\kappa = -1$) quasidiscrete level and its width $\gamma(Z, R)$ for the cutoff radius $R = 0.031$ vary. The position of the S -matrix pole corresponds (for $Z = 232$) to the energy resonance $\epsilon^* = 4.85$, and $\gamma^* = 0.09$ to the resonance width. This agrees with Fig. 2, where the phase $\delta^* = 1.67$ corresponds to the positron energy ϵ^* , and the resonance width falls into the region of the fast variation of the phase.

⁴ The same ‘wrong’ sign in front of the imaginary part of the energy for $Z > Z_{cr}$ was obtained previously in Refs [11, 12].

⁵ In Refs [35, 36], the solutions of the Klein–Fock–Gordon and the Fock equations in the framework of the effective radius approximation are compared in terms of the trajectories of scattering matrix poles near the lower continuum boundary. A qualitative difference between these two problems was noted in [10].

With modification (11) of the Coulomb potential, the Hamiltonian $H_D(r; \kappa; R)$ becomes self-adjoint, and its eigenfunctions form a complete system, i.e., a basis. Because the electron spectrum $-1 < \varepsilon < \infty$ and the positron spectrum $0 \leq \varepsilon_p < \infty$, $\varepsilon_p = -\varepsilon$ for $\varepsilon \leq -1$ do not overlap,⁶ Furry's quantization procedure [37] using this basis is applicable. Importantly, for the complex energy of a positron quasistationary state, we have

$$\varepsilon_{ps} = \varepsilon_0 - \frac{i}{2} \gamma, \quad \varepsilon_0 > 0, \quad \gamma > 0, \quad (29)$$

which is the usual expression for the energy of a quasidecrete level (for $Z > Z_{cr}$, the resonance scattering of a positron, albeit on a supercritical atom, was briefly discussed in [20]). The above quantization is consistent for any value of the charge, and hence there is no reason to expect the nuclear charge to be screened at $Z > Z_{cr}$ by vacuum-produced pairs (as discussed in Refs [11, 12, 14–25]).

Mathematically, the assertion of no spontaneous e^+e^- pair production follows from the fact that in the problem we are considering, the in- and out-states with a given quantum number κ are unitarily equivalent because scattering matrix (22), $S_\kappa(k; Z) = \exp(2i\delta(k; Z))$, is unitary due to the real-valuedness of the scattering phase (see Fig. 2). This is where the supercritical Coulomb problem differs considerably from the problem of the Klein paradox [38], where positive- and negative-frequency states overlap and two complete solution sets of the Dirac equation (the in- and out-sets) must be used [39–42].

6. Conclusion

The ‘cutoff’ procedure [10], i.e., the Coulomb potential regularization at short distances, ensures the self-adjointness of the Dirac Hamiltonian and hence determines a complete set of orthonormal solutions of the radial Dirac equation for any nucleus charge Z . This implies that the one-particle approximation for the Dirac equation is consistent not only for $Z < Z_{cr}$ but also for the supercritical region $Z > Z_{cr}$, thus implying that a bare supercritical nucleus is stable in the vacuum. We note that corresponding to the vacuum, i.e., to the lowest-energy state, are the unfilled states of the upper continuum, the unfilled discrete levels, and the states (fully occupied by electrons) of the lower continuum (the Dirac sea distorted by the presence of a heavy $Z > Z_{cr}$ nucleus). By the Pauli principle, e^+e^- pair production from the vacuum by a supercritical Coulomb field is impossible because the electron of a pair cannot occupy an already occupied state in the Dirac sea, and therefore the supercritical atom that was discussed in Refs [20, 23] cannot form. In the framework of Furry's secondary quantization procedure, the states corresponding to the Dirac sea are unoccupied positron states, and those corresponding to the vacuum are no-particle states.

We discuss the question, addressed in Ref. [10], of what happens to the electron of a hydrogen-like atom when the nucleus charge exceeds the critical value. If the charge changes as a result of a proton or an α particle being absorbed by the nucleus, then the question reduces to the standardly solvable problem of atom ionization by ‘shake-up’ [43]. In this case, a bound ‘undercritical’ electron can be found with different probabilities in the electron states of the

discrete and continuous spectra of the supercritical nucleus, and therefore a $Z > Z_{cr}$ ion does not have the specific properties of a ‘supercritical’ ion as described in [20].

For a charge changing adiabatically near $Z = Z_{cr}$, screening due to the vacuum polarization, i.e., the change in the shape of the electrostatic potential, should be taken into consideration, making the problem a many-particle one. The adiabatic increase in the effective charge occurs in the collision of two nuclei, but this is already a completely different problem, the subject of many experimental and theoretical studies (for more on this, see Ref. [44]). We note that e^+e^- pair production due to two heavy nuclei approaching each other was recently treated in the standard quantum electrodynamics framework in [45].

We finally note that all the above-mentioned aspects of the supercritical Coulomb problems arise in the nonrelativistic theory of two-dimensional impurity heterostructures. For example, the electronic properties of SiC-substrated graphene doped with light nuclei or ions are described in terms of an effective two-dimensional gapped Dirac equation [27, 46]. The energy spectrum in such a two-dimensional Coulomb problem is determined by Dirac system (1) with the replacement $\kappa \rightarrow -J$, where J is the total conserved two-dimensional angular momentum, which can take any negative or positive value (including half-integer values $J = 0, \pm 1/2, \pm 1, \pm 3/2, \dots$) and can also be zero [27]. All the questions raised above can be answered by measuring the energy levels in graphene doped with charged impurities.

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7. Appendix

The term ‘critical nuclear charge $Z_{cr}e$ ’ usually refers [10] to the value of Ze for which the level $E_d = \varepsilon_d mc^2$ of the discrete spectrum lowers to the boundary of the lower solution set of the Dirac equation:

$$\varepsilon_d(k, Z_{cr}a) = -mc^2 \quad (A.1)$$

(we set $\hbar = c = m = 1$ hereafter). Below is a brief discussion of how to calculate Z_{cr} .

Solving Dirac equation (15) with the Coulomb potential $V(r) = -Z\alpha/r$ for the energy $\varepsilon_d = -1$ is quite straightforward because, in this case, $\rho = 2\lambda r \rightarrow 0$, $a \rightarrow \infty$, and the identities

$$\lim_{a \rightarrow \infty} \left[\Gamma(a - c + 1) \Psi\left(a, c, \frac{x}{a}\right) \right] = 2\sqrt{x^{1-c}} K_{c-1}(2\sqrt{x}),$$

$$\Psi'(a, c, x) = \frac{1}{x} [(a - c + x)\Psi(a, c, x) - \Psi(a - 1, c, x)]$$

hold (see the reference book [33]). We note that

$$F(r) = K_{iv}(\sqrt{8Z\alpha r}), \quad G(r) = \frac{1}{Z\alpha} \left(r \frac{d}{dr} + \kappa \right) F, \quad (A.2)$$

$$F, G \sim r^{\mp 1/4} \exp(-\sqrt{8Z\alpha r}), \quad r \rightarrow \infty, \quad (A.3)$$

where $v = 2[(Z\alpha)^2 - \kappa^2]^{1/2} > 0$, $\kappa = \mp(j + 1/2)$, $j = 1/2, 3/2, \dots$, κ is an integral of motion of the Dirac equation in a

⁶ This also remains true for $Z = Z_{cr}$ when the energy $\varepsilon_d = -1$ corresponds to a bound electron state and $\varepsilon_p > 0$.

central field, $K_{iv}(z)$ is the Macdonald function,⁷ and F and G are the radial wave functions for the respective upper and lower components of the Dirac bispinor.

Expression (A.2) is valid for $\varepsilon_d = -1$ and $r > R$; in the range $0 < r < R \ll 1$, the potential $V(r)$ differs from the Coulomb potential because of the finite nucleus size. Neglecting terms of the order of $R \ll 1$ and matching wave functions at the edge of the nucleus, we obtain the equation for the critical charge Z_{cr} [11, 12],

$$\frac{zK'_{iv}(z)}{2K_{iv}(z)} = \xi, \quad (\text{A.4})$$

where $z = 2\sqrt{2Z_{\text{cr}}\alpha R}$, and

$$\xi = \frac{r}{F} \left(\frac{dF}{dr} \right)_{r=R} = \begin{cases} \frac{Z\alpha}{\tan(Z\alpha)}, & \kappa = -1, \\ \frac{(Z\alpha)^2 \tan(Z\alpha)}{\tan(Z\alpha) - Z\alpha}, & \kappa = 1 \end{cases} \quad (\text{A.5})$$

is the dimensionless logarithmic derivative [the last expressions refer to the rectangular cutoff model (11)]. The numerical solution of Eqns (A.4) and (A.5) yields the values of Z_{cr} listed in Table 1. A more realistic cutoff model,

$$V(r) = \begin{cases} -\frac{Z\alpha}{2R} \left[3 - \left(\frac{r}{R} \right)^2 \right], & 0 < r < R, \\ -\frac{Z\alpha}{r}, & r > R, \end{cases} \quad (\text{A.6})$$

which corresponds to a nucleus with a constant volume charge density, yields the respective values $Z_{\text{cr}}(1s_{1/2}) = 168, 170, 173$ for $r_0 = 8, 10, 12$ F [11, 12]. We also note that extrapolating the dependence $r_0 = 1.2A^{1/3}$ [F], $A = 2.5Z$ common to heavy nuclei to the region $Z > 137$ yields $Z_{\text{cr}}(1s_{1/2}) = 169$ for the ground state.

Setting $\varepsilon = -1$ in Eqn (17) for the energy spectrum with $Z\alpha > |\kappa|$, we obtain Eqn (18) for the critical charge for which the level with a given κ reaches the boundary of the lower continuum. The solutions of this equation obtained using equality (14) resulting from cutoff model (11) are listed in Table 1 for different values of the cutoff radius R .

Although markedly different in their form, Eqns (A.4) and (18), (14) for the critical nuclear charge produce similar values of Z_{cr} (see the tabulated values for the lowest levels $nS_{1/2}$ and $np_{1/2}$), thus providing independent support to the method developed in this paper.

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⁷ The function K_{iv} takes real values for $0 < z, v < \infty$ and has the asymptotic forms $K_{iv}(z) = \sqrt{\pi/[v \sinh(\pi v)]} \sin[v \ln(2/z) + \arg \Gamma(1+iv)]$ as $z \rightarrow +0$ and $K_{iv}(z) = \exp(-z)\sqrt{\pi/(2z)}[1 - (v^2 + 1/4)/2z]$ as $z \rightarrow \infty$.