On solutions of the Dirac equation in a strong disappearing at infinity electrostatic field

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Abstract. It is shown that the one-particle radial Dirac equation with a spherically symmetric narrow rectangular well remains valid also in the supercritical region. Positron resonances in scattering arising at low supercriticality are in no way related to the process of spontaneous production of electron-positron pairs from vacuum.

1. Introduction
The question of the validity of the one-particle Dirac equation in a strong electrostatic field disappearing at infinity was apparently first posed in the work of Schiff, Snyder, and Weinberg [1]. Using the example of a spherically symmetric rectangular potential well of depth $V_0$ they showed, that as the $V_0$ increases, the electron levels move from the bottom of the upper continuum of the Dirac equation solutions to the upper boundary of the lower continuum. However, the authors of [1] believed that for sufficiently large $V_0$ the vacuum is not a state with the lowest energy of the system, but differs from it by finite values of the charge and energy.

In greater detail, for any values of $\kappa$, this problem is considered in the monograph [2], moreover the cases of both a narrow and a wide well (comparing to the Compton wavelength of the electron $l_C = \hbar/mc$) are discussed. Just as in [1], it is noted that the difficulty of interpretation arises when $V_0$ exceeds the so-called “critical” value $V_{cr}$, at which the given level reaches the boundary of the lower continuum. It is claimed, by analogy with the relativistic Coulomb problem with the charge of a nucleus $Z > Z_{cr}$ [3,4], that this difficulty is due to spontaneous production by the field at $V_0 > V_{cr}$ of electron-positron pairs, so that the problem “cannot be solved within the framework of the quantum mechanics of a single particle”.

At the same time, papers [5–8] show arguments based on the general principles of quantum theory that the one-particle Dirac equation remains valid also in the region of supercritical fields. In particular, at a small supercriticality, resonance scattering of positrons by the nucleus occurs. Nevertheless, the authors of the work [9] disagree with this conclusion and consider that resonances in scattering of positrons by the supercritical nucleus indicate spontaneous production of electron-positron pairs at $Z > Z_{cr}$.

In the present article we show that in the model of a spherical rectangular well used in [1] the one-particle Dirac equation remains valid also in the supercritical region.

1 The paper [1] discussed levels with a Dirac quantum number $\kappa = \mp 1$. 
2. The scattering phase and the poles of the scattering matrix of $s$-states

The radial Dirac equation of states with a conserved Dirac quantum number $\kappa = \pm 1, \pm 2, \ldots$ in units of $\hbar = c = m = 1$ takes the form

$$
H_D \Psi_{\varepsilon, \kappa}(\rho) = \varepsilon \Psi_{\varepsilon, \kappa}(\rho), \quad \Psi_{\varepsilon, \kappa} = \begin{pmatrix} F(\rho) \\ G(\rho) \end{pmatrix}, \quad \varepsilon = E/mc^2, \quad \rho = r/l_C,
$$

$$
H_D = \begin{pmatrix} V(\rho) + 1 - \frac{d}{d\rho} - \frac{\varepsilon}{\rho} & \frac{d}{d\rho} - \frac{\varepsilon}{\rho} \\ - \frac{d}{d\rho} - \frac{\varepsilon}{\rho} & V(\rho) - 1 \end{pmatrix}, \quad \varepsilon = -(l + 1), -\tilde{l}, \quad j = |\kappa| - 1/2,
$$

$$
\kappa = \pm \frac{1}{2}, \quad l, \tilde{l} + 1, \quad j = \kappa - 1/2.
$$

(1)

Here, $j$ is the total angular momentum, and $l$ and $\tilde{l}$ are the orbital angular momenta of the upper and lower components of the Dirac spinor $\Psi_{\varepsilon, \kappa}$, respectively.

For the potential

$$
V(\rho) = -\theta(R - \rho)V, \quad V = V_0/mc^2,
$$

(2)

where $\theta(x)$ is the Heaviside step function, equation (1) is solved in Bessel functions. So, for example, for the partial elastic scattering phase $\delta_{\varepsilon}(k)$ in states with $\kappa = -1$ we have

$$
\delta_{-1}(k) = \delta^{(s)}(k) - kR, \quad \cot \delta^{(s)}(k) = \frac{1}{kR} \left\{ 1 - \frac{(\varepsilon + 1)}{(V + \varepsilon + 1)} \left[ 1 - \kappa R \cot(\kappa R) \right] \right\},
$$

(3)

where $\kappa = \sqrt{(V + \varepsilon)^2 - 1}$ and $k = \sqrt{\varepsilon^2 - 1}$ are the wavevectors of the particle inside and outside the well. The poles of the partial elastic scattering matrix $S_{\varepsilon}(k)$ is solved in Bessel functions. The equation $\cot \delta^{(s)}(i\lambda) = i$, determines the discrete spectrum of the problem, which for $\kappa = -1$ gives the equation for the spectrum of $ns_1/2^2$-states,

$$
\kappa R \cot(\kappa R) = -\lambda R - \frac{V}{(\varepsilon + 1)}(1 + \lambda R), \quad \lambda = \sqrt{1 - \varepsilon^2}, \quad -1 \leq \varepsilon \leq 1.
$$

(4)

In the case of a narrow well, $R \ll 1$, this equation can be represented in the form:

$$
V = \frac{n\pi}{R} - (2\varepsilon + 1) + \left[ (1 + \varepsilon) \sqrt{1 - \varepsilon^2} + \frac{1}{2n\pi} \right] R + O(R^2),
$$

(5)

$n = 1, 2, \ldots$ is the radial quantum number. By taking $\varepsilon = -1$ and $n = 1$ in (5), we obtain the critical value of the depth of the well for the ground state,

$$
V_c^{(s)}/mc^2 \equiv V_c^{(s)} = \frac{\pi}{R} + 1 + \frac{1}{2\pi} R + O(R^2),
$$

(6)

which is consistent with the result [5]. When $V > V_c^{(s)}$, the level dives into the lower continuum, turning into a quasistationary state with complex energy. To determine it, one can use the equation (4), which is convenient to represent near the lower continuum boundary in the form [5]

$$
V_c^{(s)} - V = a_2^{(s)} \lambda^2 + a_3^{(s)} \lambda^3,
$$

(7)

where, $a_2^{(s)} = 1 - R/2\pi$, $a_3^{(s)} = -R/2$ for $n = 1$ and $R \ll 1$.

An analytic continuation to the domain $V > V_c^{(s)}$, $\lambda = -ik$ gives

$$
k_\pm = k_\pm' - ik'', \quad k_\pm' = \pm (1 + R/4\pi)(V - V_c^{(s)})^{1/2}, \quad k'' = \frac{1}{4} R(V - V_c^{(s)}).
$$

(8)
Figure 1. The $S$-matrix poles motion in the complex $k$-plane near the boundaries of the lower (a) and upper (b) continua for $\kappa = -1$ and $R = 1/5$. The marks denotes the values of $(V - V_c^{(s)})$ and $(V_b^{(s)} - V)$, respectively.

Figure 2. Scattering phases near the boundary of the lower continuum for $\kappa = -1$ and $R = 1/20$. The shaded area shows the position and the width of the Breit–Wigner resonances. The numbers denotes the values of $(V - V_c^{(s)})$.

The motion of the poles of the matrix $S_{-1}(k)$ in the complex $k$-plane as a function of $(V - V_c^{(s)})$ is shown in Fig. [1]. The pole closest to the physical region will be called a Breit–Wigner pole, $k_+ = k_{BW}$. The energy of such an $s_{1/2}$-level in the lower continuum, $\varepsilon_{BW} = -\sqrt{k_{BW}^2 + 1}$, is

$$\varepsilon_{BW}^{(s)} = -\varepsilon^{(s)} + \frac{i}{2} \gamma^{(s)}, \quad \varepsilon^{(s)} = 1 + \frac{i}{2} \left(1 + R/2\pi\right) (V - V_c^{(s)}), \quad \gamma^{(s)} = \frac{i}{2} R (V - V_c^{(s)})^{3/2}. \quad (9)$$

An unusual sign of the imaginary part, $\gamma^{(s)} > 0$, is coming from the use of a nonsecond-quantized approach. The Breit–Wigner level $\varepsilon_{BW}^{(s)}$ in the Dirac sea corresponds to the quasistationary state of the positron with energy

$$\varepsilon_{qs}^{(s)} = -\varepsilon_{BW}^{(s)} = \varepsilon^{(s)} - \frac{i}{2} \gamma^{(s)}, \quad \varepsilon^{(s)} > 0, \quad \gamma^{(s)} > 0, \quad (10)$$

which has the correct sign of the imaginary part.

At a small supercriticality, this quasidiscrete level manifests itself as a Breit–Wigner resonance in the elastic scattering of a positron with a width $\gamma^{(s)}$. The threshold behavior of the width is determined by the permeability of the centrifugal barrier,

$$D \sim k^{2L+1}, \quad k \to 0. \quad (11)$$
Near the boundary of the lower continuum one must take \( [5] \) the orbital angular momentum \( \tilde{l} \) of the lower component of (1) as the orbital angular momentum \( L \). In the case under consideration, \( L = \tilde{l} = 1 \), which agrees with the result \( [6] \) for the width \( \tilde{\gamma}^{(s)} \). The phase of elastic scattering of the positron as a function of its energy \( \tilde{\varepsilon} = -\varepsilon \) is shown in Fig. 2. It is seen that at an energy \( \varepsilon \) close to the position of the resonance \( \tilde{\varepsilon} = \varepsilon \), the phase changes abruptly on the width \( \tilde{\gamma}^{(s)} \).

Similarly, one can consider the motion of the poles of \( S_{-1}(k) \) near the boundary of the upper continuum. However, as opposed to (7), here the expansion begins with a linear term,

\[
V - V_b^{(s)} = c_1^{(s)} \lambda + c_2^{(s)} \lambda^2, \quad c_1^{(s)} = 2R, \quad c_2^{(s)} = 1 + \frac{3}{2\pi} R, \quad V_b^{(s)} = \frac{\pi}{R} - 3 - \frac{3}{2\pi} R, \tag{12}
\]

and the first bound level appears at \( V = V_b^{(s)} \). Putting \( \lambda = -ik \) in (12), we obtain

\[
k_{\pm}^{(s)} = \pm iR \sqrt{(1 + \frac{3}{2\pi} R)(V - V_b^{(s)})/R^2 + 1} - iR. \tag{13}
\]

As the depth of the well decreases, the discrete level \( k_{q}^{(s)} = k_{i}^{(s)} \) moves downward along the positive imaginary axis of the \( k \)-plane. At \( V = V_b^{(s)} \), it reaches the boundary of the upper continuum, and with a further decrease of \( V \) it is “pushed” into it, turning into a virtual, rather than quasistationary, level \( k_{v}^{(s)} \), since \( l = 0 \) and there is no centrifugal barrier. At the same time, a second virtual level \( k_{v}^{(s)} \) moves towards it, for which \( k_{v}^{(s)} = -2iR \) at \( V = V_b^{(s)} \). When \( V = V_b^{(s)} - R^2 \), they collide, then they go to the complex plane, see Fig. 1b.

3. The scattering phase and the poles of the scattering matrix of \( p \)-states

For \( np_{1/2} \)-states, i.e. at \( \kappa = 1 \), the discrete spectrum is determined by the equation

\[
\kappa R \cot(\kappa R) = -\lambda R + \frac{V}{(1 - \varepsilon)(1 + \lambda R)}, \quad \lambda = \sqrt{1 - \varepsilon^2}, \quad -1 \leq \varepsilon \leq 1. \tag{14}
\]

which for \( R \ll 1 \) is equivalent to the equality

\[
V = \frac{n\pi}{R} - (2\varepsilon - 1) - \left[ (1 - \varepsilon) \sqrt{1 - \varepsilon^2} - 1 - 2\varepsilon(\varepsilon - 1) \right] R + O(R^2). \tag{15}
\]

The first bound \( 1p_{1/2} \)-level appears at \( V = V_b^{(p)} \),

\[
V_b^{(p)} = \frac{\pi}{R} - 1 + \frac{1}{2\pi} R + O(R^2), \tag{16}
\]

and equation (14) for \( V - V_b^{(p)} \ll 1 \) can be represented in the form

\[
V - V_b^{(p)} = a_2^{(p)} \lambda^2 + a_3^{(p)} \lambda^3, \quad a_2^{(p)} = 1 - R/2\pi, \quad a_3^{(p)} = -R. \tag{17}
\]

Comparison with the expansion \( [7] \) shows that the motion of the poles of the \( S \)-matrix at \( \kappa = 1 \) near the boundary of the upper continuum with decreasing \( V \) is similar to the motion of the poles of the \( S \)-matrix at \( \kappa = -1 \) in the vicinity of \( \varepsilon = -1 \) with increasing \( V \), cf. Fig. 1a.

For the energy of the quasistationary Breit–Wigner state of the electron, we obtain

\[
\varepsilon_{qs}^{(p)} = \varepsilon_{BW}^{(p)} = \varepsilon^{(p)} - \frac{i}{2} \gamma^{(p)}, \quad \varepsilon^{(p)} = 1 + \frac{1}{2} (1 - \frac{1}{2\pi} R) (V_b - V), \quad \gamma^{(p)} = R(V_b - V)^{3/2} > 0. \tag{18}
\]
The results obtained above for the cases \( \kappa \approx 1 \) near the boundary of the lower continuum is analogous to the motion of the poles with \( \kappa = -1 \) for \( \varepsilon \sim 1 \). In this case, Eq. (15) gives

\[
V_c^{(p)} - V = c_1^{(p)} \lambda + c_2^{(p)} \lambda^2, \quad c_1^{(p)} = 2R, \quad c_2^{(p)} = 1, \quad V_c^{(p)} = \frac{\pi}{R} + 3 \frac{3}{2\pi} R,
\]

and the signs of the coefficients \( c_1^{(p)} \) and \( c_2^{(p)} \) are just such that for \( V > V_c^{(p)} \) the level goes to the second, unphysical sheet [6]. Indeed, setting \( \lambda = -ik \), we obtain

\[
k_{\pm}^{(p)} = \pm i \sqrt{(V_c^{(p)} - V) + R^2 - iR}.
\]

For \( V < V_c^{(p)} + R^2 \), the real level, with increasing \( V \), moves down the imaginary axis of the \( k \)-plane, becoming a virtual level at \( V_c^{(p)} < V < V_c^{(p)} + R^2 \). The second virtual level moves towards it. When \( V = V_c^{(p)} + R^2 \), they collide, going to the complex plane. And the level which moves to the right, being closer to the physical region, has the energy

\[
\tilde{\varepsilon}^{(p)}_\pm = -\tilde{\varepsilon}^{(p)} + \frac{i}{2} \tilde{\gamma}^{(p)}, \quad \tilde{\varepsilon}^{(p)} = -1 - \frac{1}{2} (V - V_c^{(p)}), \quad \tilde{\gamma}^{(p)} = R (V - V_c^{(p)})^{1/2}.
\]

For the energy of the quasidiscrete level of the positron in the state \( p_{1/2} \), we get:

\[
\tilde{\varepsilon}_v^{(p)} = -\tilde{\varepsilon}_-^{(p)} = \tilde{\varepsilon}^{(p)} - \frac{i}{2} \tilde{\gamma}^{(p)}, \quad \tilde{\varepsilon}^{(p)} > 0, \quad \tilde{\gamma}^{(p)} > 0.
\]

The dependence of the width \( \tilde{\gamma}^{(p)} \) on supercriticality is determined in this case by the orbital angular momentum \( l = 0 \), which means the absence of a centrifugal barrier.

4. The case of arbitrary values of the Dirac quantum number \( |\kappa| \gg 2 \)

The results obtained above for the cases \( \kappa = \mp 1 \) are generalized to arbitrary values \( |\kappa| \gg 2 \). For energies of the Breit–Wigner resonances near \( \varepsilon = 1 \), i.e. for quasistationary electron states, we have

\[
\tilde{\varepsilon}_{qs}^{(x)} = \tilde{\varepsilon}_{BW}^{(x)} = \tilde{\varepsilon}^{(x)} - \frac{i}{2} \tilde{\gamma}^{(x)}, \quad \tilde{\varepsilon}^{(x)} > 1, \quad \tilde{\gamma}^{(x)} > 0,
\]

with \( \gamma^{(x)} \sim (V_b^{(x)} - V)^{1+1/2} \), \( l = j + \frac{1}{2} \text{ sgn } \kappa \).

At the same time, near the lower continuum boundary for the Breit–Wigner energy follows:

\[
\tilde{\varepsilon}_{BW}^{(x)} = -\tilde{\varepsilon}^{(x)} + \frac{i}{2} \tilde{\gamma}^{(x)}, \quad \tilde{\varepsilon}^{(x)} > 1, \quad \tilde{\gamma}^{(x)} > 0,
\]

with the threshold dependency \( \tilde{\gamma}^{(x)} \sim (V - V_c^{(x)})^{1+1/2} \), \( \tilde{l} = j + \frac{1}{2} \text{ sgn } \kappa \). We note that the inequality \( \tilde{\gamma}^{(x)} > 0 \) holds for a well of arbitrary shape, as shown in [6] within the framework of the effective radius approximation for the Dirac equation developed there.

An invalid sign in front of \( \tilde{\gamma}^{(x)} \) in (24) means the need for a second quantization. The Dirac radial Hamiltonian [1] with potential [2] is a self-adjoint operator whose solutions form a complete system of functions. According to Furry, it can be used to quantize the system [10].

In the Furry picture, the solutions of the Dirac equation in the lower continuum correspond to positron states with energy \( \varepsilon = -\varepsilon > 1 \). Therefore, the Breit–Wigner poles (24) match the quasistationary positron states with energy having a negative imaginary part,

\[
\tilde{\varepsilon}_{qs}^{(x)} = -\tilde{\varepsilon}_{BW}^{(x)} = \tilde{\varepsilon}^{(x)} - \frac{i}{2} \tilde{\gamma}^{(x)}, \quad \tilde{\varepsilon}^{(x)} > 1, \quad \tilde{\gamma}^{(x)} > 0.
\]
With a small supercriticality, this leads to resonance scattering of positrons.

Due to the fact that the partial scattering phases $\delta_{\kappa}(k)$ are real, the elastic scattering matrix of positrons $S_{\kappa} = \exp[2i\delta_{\kappa}(k)]$ is unitary. Thus, inelastic processes in the channel with given $\kappa$, including spontaneous $e^+e^-$-pair production, are absent.

Thereby, the resonance scattering of positrons at small supercriticality, analogous to the resonance scattering of electrons at small underboundness, can not serve as evidence in favor of the spontaneous production of electron-positron pairs. This is the essential difference between strong electrostatic fields that disappear at infinity and the situation that arises in the Klein paradox \cite{11}, or in a constant uniform electric field.

5. Conclusions
As a result, the one-particle approximation for the Dirac equation in the field of a spherically symmetric narrow rectangular well remains valid also in the region of the supercritical depths of such a well. In this model, the discrete levels are well separated from each other near the boundary of both the lower and the upper continua. Therefore, it is not difficult to consider the motion of the poles of the scattering matrix in the vicinity of these boundaries.

At present, a large number of both theoretical and experimental works are devoted to the Coulomb problem in graphene, the dynamics of charge carriers in which is described by the effective two-dimensional Dirac equation in the presence of an impurity with a charge $Z$, including in the supercritical case, $Z > Z_{cr}$. Moreover, it was shown in Refs. \cite{12,13} that the positions of the resonances calculated in the gapless equation agree with the experimental data on the spectra of current-voltage characteristics obtained by scanning tunneling microscopy. This means the validity of the one-particle effective gapless two-dimensional Dirac equation for $Z > Z_{cr}$, but the discussion of this question is beyond the scope of this article.

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