Simple model of scalar-vector interaction for the relativistic two-center problem

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The ground-state wave function and the energy term of a relativistic electron moving in the field of two fixed centers, when interaction of this particle with centers is described by two Coulomb and two Coulomb-like scalar potentials are calculated analytically by the linear combination of atomic orbitals method. By means of perturbation theory the asymptotic expansions (at small and large internuclear distances R) of the eigenvalues $E(R)$ of the system for arbitrary states are obtained. The dependence of critical charge Z_{cr} and critical distance R_{cr} from the scalar coupling constant was investigated.

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I. INTRODUCTION

The motion of an electron in the field of two Coulomb centers (at a fixed distance R) is one of the fundamental problem in quantum mechanics, which continues to attract the interests of theoretical physicists. The nonrelativistic two-Coulomb-center problem has been investigated thoroughly in [1–3] (see references therein). The two-center Dirac equation was solved for the first time by Müller and Greiner [4]. There are various approximations for solving the Dirac equation for the two-Coulomb-center problem [5–8].

In this paper, we wish to discuss the relativistic two-center problem with Coulomb vector and Coulomb-like scalar potentials. There has been considerable interest in studying the behavior of quantum systems of fermions at the presence of electromagnetic (vector) and scalar external fields (see, for example, [9–13], and references therein). These systems have a number of extraordinary features, which essentially do not exist in the case of the presence of the electromagnetic field only.

The Dirac equation has the following form at the presence of static scalar $\hat{S}(\vec{r})$ and electrostatic $\hat{V}(\vec{r})$ external fields

$$\{c\vec{\alpha}\cdot\hat{\vec{p}}+\beta[m_0c^2+\hat{S}(\vec{r})]+\hat{V}(\vec{r})\}\Psi(\vec{r})=E\Psi(\vec{r}). \qquad (1)$$

Let us point out that $\hat{S}(\vec{r})$ is a Lorentz scalar, and $\hat{V}(\vec{r})$ is the zero component of a Lorentz vector. The solution and spectrum of the Dirac equation for the simple model of the interaction of fermions with Coulomb-like scalar and vector external fields,

$$\hat{S}(r)=-\hbar c\frac{\alpha_S}{r}, \quad \hat{V}(r)=-\hbar c\frac{\alpha_V}{r}, \qquad (2)$$

have been found in Refs. [14,15]. In Eq. (2) α_S and α_V are the scalar and electrostatic coupling constants, respectively.

It is significant that in the context of mixed scalar-vector models the interaction between leptons and nuclei is carried out by the exchange of two different types of a field quantum. Namely, if the Coulomb interaction is conditioned by the exchange of a virtual photon (by the quantum of an electromagnetic field), the corresponding scalar interaction of a lepton with a nuclei can be caused by the exchange of a virtual neutral particle with spin 0. The main candidate for this role is the scalar σ meson. There are serious theoretical arguments (see, for example, [16], and references therein) in the favor of existence of this particle. It should be mentioned here that the idea of the existence of such a scalar meson presumably was first expressed in 1959 [17]. However, it is important to note that in 1934 De Broglie considered the existence of a massive "scalar photon" [18]. Recently, two experimental groups have reported [19,20] the observation of an anomalous wide scalar resonance in the cascades of nonleptonic decays of heavy (D, B, and J/V) mesons. In these experiments the scalar meson has large mass ($M=390$ MeV [19–21]), and therefore the scalar potential which corresponds to the exchange of such a particle (potential of one-meson exchange) is actually short range (a Yukawa-type potential). Nevertheless, as noted in [14,15] and [22] within the framework of such a relatively simple model with the scalar-vector variant of the interaction [the examined model (2)], it is possible to find many interesting features of the spectrum of leptonic atoms, which would exist in more realistic models. The simple model (2) describes the exchange of a virtual massless neutral particle with a spin-0 photon ("scalar photon") and a virtual photon ("vector photon"). A similar model has been considered for the description of interaction between a fermion and an antifermion [23]. It should be stressed that the possibility of low-energy zero-spin photon generation from high-energy γ-ray photons in pair production has been studied in [24].

As it is well known (see [25,26]) that the essential theoretical parameters in the electrodynamics of super-strong Coulomb fields are the critical charge of a nucleus Z_{cr} and the critical distance R_{cr} in the system of two colliding heavy nuclei. If these parameters are attained, the ground level of the electron spectrum descends to the boundary of the lower continuum. Afterwards, i.e., at $Z=Z_1+Z_2>Z_{cr}$ or $R<R_{cr}$, the spontaneous generation of positrons from the vacuum becomes possible. The experimental observation of this effect would mean the verification of the status of QED and the Dirac equation in the new region of super-strong fields, rather than in the traditional direction of super high energies

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and small distances. Such experiments started almost one-quarter of the century ago at GSI (Darmstadt, Germany) on the accelerator of heavy ions UNILAC; however, they gave no positive result in the search for this fundamental process. In view of such a situation, a number of theorists [15,27] have considered different modifications of QED and their influence on the spontaneous generation of positrons. In this connection, we would like to investigate a question on influence of additional Coulomb-like scalar potential on Z_{cr} and R_{cr}.

We should note that Eq. (1) with the potential (2) can be used for describing the motion of a relativistic particle with spin-1/2 and position-dependent mass $m^*(r)=m_0(1-\alpha_S\lambda_c/r)$, where λ_c is the Compton wavelength. Similar approach has been used to study the motion of the relativistic particle with position-dependence mass in external fields [28]. Wave equations with a position-dependent mass play an important role in many physical problems. They appear in the energy-dependent functional approach to quantum many-body systems (e.g., nuclei, quantum liquids, ^{3}He clusters, and metal clusters) and are very useful in the description of electronic properties of condensed-matter systems [29] (e.g., compositionally graded crystals, quantum dots, and liquid crystals).

II. ENERGY OF RELATIVISTIC TWO-CENTER SYSTEM WITH SCALAR-VECTOR INTERACTION

A. Linear combination of atomic orbitals method

One of the simplest methods of calculating the energies of electron states in molecules is the approximation of wave functions by a linear combination of atomic orbitals [(LCAO) method] centered on the atoms. In the simplest form of this method, only a single atomic orbital is used in the calculation of the electron states; one can then simply obtain many interesting properties: such as the energy of a state having arbitrary translational symmetry, the density of states as a function of energy, and the charge density of the electrons between the atoms [30].

The idea of optimizing the atomic orbitals used in the LCAO method has previously been applied to calculations on atoms and molecules. It has already been used by Finkelstein and Horowitz [31] in their calculations for a H_2^+ molecule. Henceforth, the LCAO method is widely used to solve the nonrelativistic [32,33] and relativistic two-center problems [34,35], which allows us to apply the LCAO method to calculate analytically the energy term for a hydrogen molecular ion and for a hydrogen molecule.

In this section we investigate the dependence of the electron binding energy of the relativistic two-center problem with potential (2) on the value of the scalar coupling constant α_S. The Dirac equation with the potential of two fixed centers (2) does not permit complete separation of variables in any orthogonal system of coordinates. Therefore, we use the modification of the LCAO method which was first proposed in [34] for the Dirac equation to find electron energy.

The distance between the nuclei is denoted by R, and the distances between the electron and the nuclei are denoted by r_1 and r_2, respectively. The motion of a relativistic electron in the field of two fixed centers is described by the time-independent Dirac equation (1) with the potentials

$$\hat{S}(\vec{r}) = -\hbar c\left(\frac{\alpha_{S1}}{r_1}+\frac{\alpha_{S2}}{r_2}\right), \quad \hat{V}(\vec{r}) = -\hbar c\left(\frac{\alpha_{V1}}{r_1}+\frac{\alpha_{V2}}{r_2}\right). \tag{3}$$

In this paper we consider the symmetric case when $\alpha_{V1}=\alpha_{V2}=\alpha_V$, $\alpha_{S1}=\alpha_{S2}=\alpha_S$. We will solve Eq. (1) with the potentials (3) within the LCAO method for the ground state by choosing the wave function in the form

$$\Psi(\vec{r}) = c_1\Psi_1(\vec{r}) + c_2\Psi_2(\vec{r}),$$

where Ψ_1 (Ψ_2) is the wave function of the electron moving in the field of the first (second) center.

From the normalization conditions $\langle\Psi_j|\Psi_j\rangle=1$ $(j=1,2)$ [32] and the fact that the ground state does not have zeroes, it follows that

$$c_1 = c_2 = \frac{1}{\sqrt{2(1+G)}},$$

where $G=\langle\Psi_1|\Psi_2\rangle$ is an overlap integral and $\langle\Psi_j|=(\varphi_j^+\chi_j^+)$, $|\Psi_j\rangle=\begin{pmatrix}\varphi_j\\ \chi_j\end{pmatrix}$.

For the functions Ψ_1 and Ψ_2, we shall take the relativistic wave functions of the atom [9,15] with Coulomb plus scalar potentials:

$$\varphi_j = Ag_j\begin{pmatrix}1\\0\end{pmatrix}, \quad \chi_j = iABg_j\begin{pmatrix}\cos\theta_j\\ e^{i\varphi}\sin\theta_j\end{pmatrix}, \quad g_j = r_j^{\gamma-1}e^{-\lambda r_j},$$

$$A = \frac{(2\lambda)^{3/2}}{2\sqrt{\pi\Gamma(2\gamma+1)}}\sqrt{\frac{(m_0c^2+E_0)(N+1)}{4m_0c^2N}}(2\lambda)^{\gamma-1},$$

$$B = \sqrt{\frac{m_0c^2-E_0}{m_0c^2+E_0}},$$

$$\lambda = \frac{\sqrt{(m_0c^2)^2-E_0^2}}{\hbar c}, \quad N = \frac{Q_Vm_0c^2+Q_SE_0}{\hbar c\lambda},$$

$$\gamma = \sqrt{1-Q_V^2+Q_S^2},$$

$$E_0 = m_0c^2\left(\frac{-Q_VQ_S+\gamma}{1+Q_S^2}\right).$$

Here Q_S and Q_V are Ritz's variational parameters. The details of the application of the variational principle to the Dirac equation are discussed in [36].

The energy of an electron can be calculated as a matrix element

$$E = \langle\Psi|\hat{H}_D|\Psi\rangle. \tag{4}$$

Substituting these wave functions into Eq. (4), we reduce the expression for the energy term to a form involving five integrals which can be expressed analytically in terms of the complete $\Gamma(x)$ and incomplete $\Gamma(x,y)$ Euler γ functions. Thus, we have

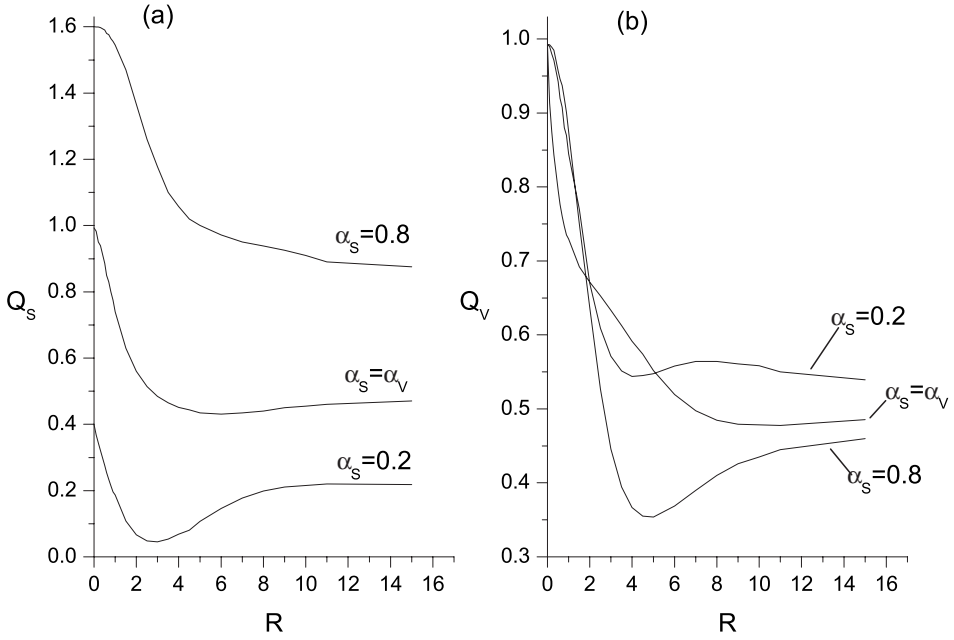

FIG. 1. (a) The variational parameter Q_S as a function of R for three different values of α_S in the case of $\alpha_V=68/137$. (b) The variational parameter Q_V as a function of R for three different values of α_S in the case of $\alpha_V=68/137$ ($\hbar=m_0=c=1$).

$$E = E_0 - \frac{4\pi A^2 (R/2)^{2\gamma}\hbar c}{1+G}[(1-B^2)(\alpha_s L - Q_S M) + (1+B^2)(\alpha_V L - Q_V M)],$$

$$L = I_2 + I_5, \quad M = \frac{I_1 + I_2}{2}, \quad I_1 = \frac{2\Gamma(2\gamma)}{a^{2\gamma}},$$

$$I_2 = \frac{1}{a^{2\gamma}}\left[\left(2 - \frac{a^2}{3(2\gamma-1)}\right)\Gamma(2\gamma,a) + \left(\frac{1}{3} + \frac{a}{3(2\gamma-1)}\right)a^{2\gamma}e^{-a}\right],$$

$$I_3 = \frac{4\gamma\Gamma(2\gamma)}{a^{2\gamma+1}},$$

$$I_4 = \frac{1}{a^{2\gamma+1}}\left[\left(4\gamma - \frac{2a^2\gamma}{3(2\gamma-1)}\right)\Gamma(2\gamma,a) + \left(2 + \frac{2a\gamma}{3(2\gamma-1)}\right)a^{2\gamma}e^{-a}\right],$$

$$I_5 = \frac{1}{a^{2\gamma+1}}\left((a-\gamma)\Gamma(2\gamma,2a) + (a+\gamma)\Gamma(2\gamma) - \frac{1}{2}(2a)^{2\gamma}e^{-2a}\right),$$

$$a = \lambda R, \quad G = 2\pi A^2(1+B^2)(R/2)^{2\gamma+1}I_4. \tag{5}$$

In the case when $\alpha_S=0$ (a pure vector coupling), $Q_S=0$ and $Q_V \to Q\alpha$, $\alpha_V \to Z\alpha$ are substituted into formula (5), we obtain

$$E = \frac{2\pi A^2 (R/2)^{2\gamma} b}{1+G}\left(Q\alpha(I_1+I_2) + \frac{a\gamma}{2Q\alpha}(I_3+I_4) - 2Z\alpha(I_2+I_5)\right),$$

$$a = Q\alpha R, \quad b = \frac{2}{1+\gamma}, \quad \gamma = \sqrt{1-Q^2\alpha^2},$$

$$G = 2\pi A^2 b (R/2)^{2\gamma+1} I_4, \tag{6}$$

where Q is an effective charge, $\alpha=1/137$ is the fine-structure constant, and Z is the electric charge of the nuclei.

Now we derive the nonrelativistic limit from Eq. (6). For $Q\alpha \ll 1$ ($\gamma \approx 1$) we have

$$E = Q^2\alpha^2 F_1(a) + Q\alpha F_2(a), \tag{7}$$

where

$$F_1(a) = \frac{1}{2}\frac{1+e^{-a}(1+a-a^2/3)}{1+e^{-a}(1+a+a^2/3)},$$

$$F_2(a) = -Z\alpha\frac{1+2e^{-a}(1+a)+1/a-(1/a+1)e^{-2a}}{1+e^{-a}(1+a+a^2/3)}.$$

Expression (7) at $Z=1$ coincides with the well-known Slater formula for the ground state of hydrogen molecular ion. So we see that formula (6) at $Q\alpha \ll 1$ ($\gamma \approx 1$) turns to formula (7), in contrast to formula (3) [34] in which error was evidently admitted.

The variational parameters Q_V, Q_S are generally functions of R, α_V, and α_S, that is $Q_{V,S}=Q_{V,S}(R,\alpha_V,\alpha_S)$. With a numerical minimization of expressions (5) we find the following behavior of variational parameters Q_V, Q_S in the limiting cases $R \to 0$ and $R \to \infty$ (results of numerical minimization are presented in Fig. 1):

$$Q_{V,S} \overset{R\to 0}{\to} 2\alpha_{V,S},$$

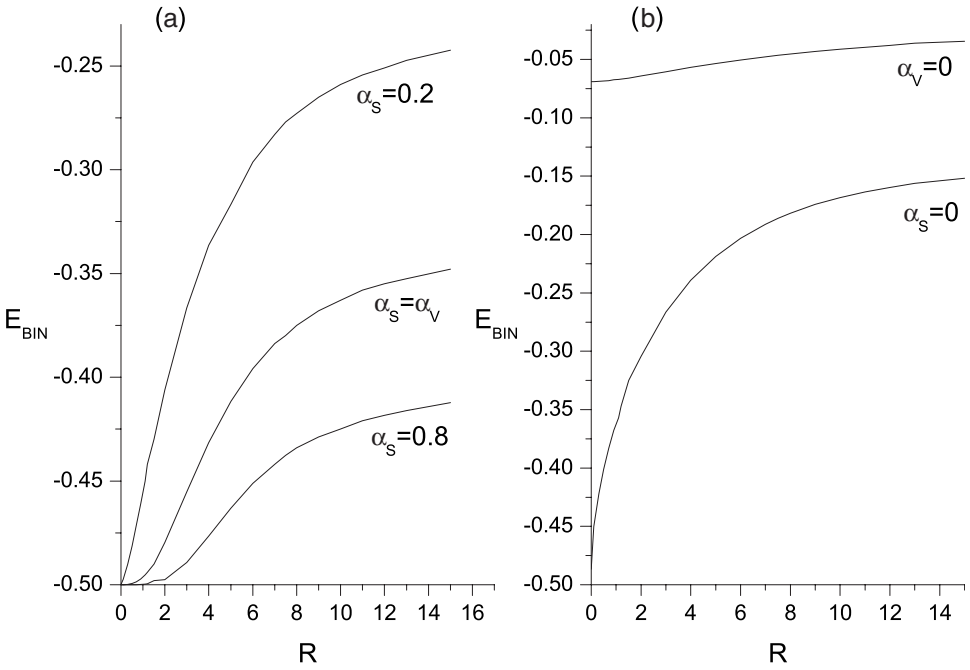

FIG. 2. (a) The ground-state binding energy of the Er^{68+}-Er^{68+} system obtained for three different values of α_S. (b) The ground-state binding energy obtained for the special cases $\alpha_S=0$ and $\alpha_V=0$ ($\hbar=m_0=c=1$).

$$Q_{V,S} \overset{R\to\infty}{\longrightarrow} \alpha_{V,S}.$$

The obtained energy term (5) is a function of R, α_V, α_S, and variational parameters Q_V and Q_S. Figure 2(a) shows the behavior of the electron binding energy of the Er^{68+}-Er^{68+} ($\alpha_V=68/137$) system as the function $E_{BIN}(R)$ of the value of the scalar coupling constant α_S. As we can see from Fig. 2(a), the binding energy increases with increasing value of α_S. It is interesting to investigate the limit cases $\alpha_S=0$ and $\alpha_V=0$. In the case of $\alpha_V=0$ ($\alpha_S=0.2$) the electron binding energy weakly depends on the internuclear distance R [see Fig. 2(b)].

Now we compare the electron energy obtained by formula (6) for H_2^+ [1(1/2)g] at the internuclear distance $R=2$ a.u. with numerical data from Table 1 of [37]. We find that our results coincide with the high accuracy data with an accuracy of 1.5%, which is a good agreement for the relatively simple method.

Finally, we have achieved analytical formula (5) for the energy term of the relativistic electron which moves in the field with the potentials (3). This formula is correct in a wide range of internuclear distances and scalar and vector coupling constants.

B. Asymptotic behavior of potential curves of two-center problem in united-atom limit

The account of an additional number of atomic orbitals in the LCAO method for calculation of the energy of the system with the potentials (3) for arbitrary level (not only in the ground state) will lead to a complication of the calculations. Therefore, it is convenient to apply asymptotic methods in some special cases. When the internuclear distance R goes to zero, it is possible to consider the relativistic two-center problem within the perturbation theory. We will examine the symmetric case when the coupling constants $\alpha_{S1}=\alpha_{S2}=\alpha_S/2$, $\alpha_{V1}=\alpha_{V2}=\alpha_V/2$ (in this section, these constants are different from the coupling constants α_V and α_S of the united atom in Sec. II A). Let us represent the Hamiltonian of the two-center problem with the potentials (3) by the sum of a Hamiltonian of zero approximation $\hat{H}^{\mathrm{UA}}$ and a perturbation $\hat{W}$,

$$\hat{H}=\hat{H}^{\mathrm{UA}}+\hat{W}. \tag{8}$$

The Dirac Hamiltonian $\hat{H}^{\mathrm{UA}}$ of the united relativistic atom is given by

$$\hat{H}^{\mathrm{UA}}=c\vec{\alpha}\cdot\hat{\vec{p}}+\beta\left(m_0c^2-\hbar c\frac{\alpha_S}{r_0}\right)-\hbar c\frac{\alpha_V}{r_0}, \tag{9}$$

where the atom is placed on the z axis at the point O which divides the internuclear distance R by one-half.

Let us introduce the spherical coordinate system $(r_0;\theta_0;\varphi_0)$: its origin is at the point O, and the angle θ_0 is measured from the z axis, which is directed from center 1 to center 2.

Now we construct the unperturbed wave function of the united atom. For the zero-order function we will choose the unperturbed wave function of the united atom with the Hamiltonian (9). The eigenvalues of the operator $\hat{H}^{\mathrm{UA}}$ are characterized by the spherical quantum numbers n, j, l, and m; where n is the principal quantum number, j and l are the total electron and orbital angular momenta, and m is the projection of j onto the internuclear axis z. The eigenfunctions of the operator $\hat{H}^{\mathrm{UA}}$ have the following form [9,15]:

$$\Psi^{\mathrm{UA}}_{njlm}(\vec{r}_0)=\begin{pmatrix} f(r_0)\Omega_{jlm}(\theta_0,\varphi_0) \\ (-1)^{1+l-l'/2}g(r_0)\Omega_{jl'm}(\theta_0,\varphi_0)\end{pmatrix}, \quad l=j\pm\frac{1}{2},$$

$$l' = 2j - l, \tag{10}$$

where Ω_{jlm} is a spherical spinor, the radial functions f and g are the large and small components of a Dirac bispinor wave function, respectively,

$$\begin{Bmatrix} f \\ g \end{Bmatrix} = \pm \frac{\sqrt{\Gamma(2\gamma + n_r + 1)}}{\Gamma(2\gamma+1)\sqrt{n_r!}} \sqrt{\frac{m_0c^2 \pm E^{\mathrm{UA}}}{4m_0c^2 N_0(N_0 - \kappa)}} (2\lambda)^{3/2}$$
$$\times (2\lambda r_0)^{\gamma-1} e^{-\lambda r_0} [(N_0 - \kappa) F(-n_r, 2\gamma+1; 2\lambda r_0)$$
$$\mp n_r F(-n_r+1, 2\gamma+1; 2\lambda r_0)], \tag{11}$$

where

$$\lambda = \frac{\sqrt{(m_0c^2)^2 - (E^{\mathrm{UA}})^2}}{\hbar c}, \quad N_0 = \frac{\alpha_V m_0 c^2 + \alpha_S E^{\mathrm{UA}}}{\hbar c \lambda},$$

$$\gamma = \sqrt{\kappa^2 - \alpha_V^2 + \alpha_S^2}, \quad n_r = n - j - \tfrac{1}{2}, \quad \kappa = \pm\left(j + \tfrac{1}{2}\right),$$

and $F(a,b;z)$ is the confluent hypergeometric function.

The eigenvalues of the operator $\hat{H}^{\mathrm{UA}}$ are determined by the formula (see, for example, [22])

$$E^{\mathrm{UA}} = m_0c^2 \left\{ \frac{-\alpha_V\alpha_S}{\alpha_V^2 + (n - j - 1/2 + \gamma)^2} + \left[\left(\frac{\alpha_V\alpha_S}{\alpha_V^2 + (n-j-1/2+\gamma)^2} \right)^2 - \frac{\alpha_S^2 - (n-j-1/2+\gamma)^2}{\alpha_V^2 + (n-j-1/2+\gamma)^2} \right]^{1/2} \right\}. \tag{12}$$

Since the spectrum of the operator $\hat{H}^{\mathrm{UA}}$ is degenerated with respect to l and m, in order to apply the perturbation theory, it is necessary to construct the exact functions of the zero approximation, for which the matrix of the perturbation operator $\hat{W}$ is diagonal. We can show that the matrix $\|W_{njlm}^{njl'm'}\|$ of the perturbation operator will be diagonal for the functions of the united atom (10) and (11). Now we determine matrix elements of the perturbation operator of the system,

$$\hat{W} = \hbar c(\alpha_V + \beta\alpha_S) \left(\frac{1}{r_0} - \frac{1}{2|\vec{r}_0 + \vec{R}/2|} - \frac{1}{2|\vec{r}_0 - \vec{R}/2|} \right).$$

For this purpose we will use the expansion of $\hat{W}$ in terms of the Legendre polynomials:

$$\hat{W} = \hbar c(\alpha_V + \beta\alpha_S) \left(\frac{1}{r_0} - \frac{1}{2} \begin{cases} \sum_{s=0}^{\infty} (-1)^s (R/2)^s r_0^{-s-1} P_s(\cos\theta_0), & r_0 > |\vec{R}/2| \\ \sum_{s=0}^{\infty} (-1)^s (R/2)^{-s-1} r_0^s P_s(\cos\theta_0), & r_0 < |\vec{R}/2| \end{cases} - \frac{1}{2} \begin{cases} \sum_{s=0}^{\infty} (R/2)^s r_0^{-s-1} P_s(\cos\theta_0), & r_0 > |\vec{R}/2| \\ \sum_{s=0}^{\infty} (R/2)^{-s-1} r_0^s P_s(\cos\theta_0), & r_0 < |\vec{R}/2| \end{cases} \right). \tag{13}$$

The coefficient of $r_0^{-2} P_1$ for $r_0 > |\vec{R}/2|$ is equal to zero. The estimates of all the radial and angular integrals with the functions (10) and (11) show that in the case of $R \to 0$, the matrix $\|W_{njlm}^{njl'm'}\|$, which has the following components,

$$W_{njlm}^{njl'm'} = \int \Psi_{njlm}^{\mathrm{UA}^+}(\vec{r}_0) \hat{W} \Psi_{njl'm'}^{\mathrm{UA}}(\vec{r}_0) dr_0,$$

is diagonal up to $O(R^3)$ with respect to each group of mutually degenerated states, i.e.,

$$W_{njlm}^{njl'm'} = \delta_{ll'}\delta_{mm'}[W_{njlm}^{njlm}]_2 + O(R^3).$$

The leading term $[W_{njlm}^{njlm}]_2$ of the expansion of the diagonal matrix element of $\hat{W}$ is determined by the expansion (13) for $r_0 > |\vec{R}/2|$, where the integration over r_0 is carried out from zero:

$$[W_{njlm}^{njlm}]_2 = -\left(\frac{\alpha_V\hbar c}{4} R^2\right) \int |\Psi_{njlm}^{\mathrm{UA}}(\vec{r}_0)|^2 r_0^{-3} P_2(\cos\theta_0) d\vec{r}_0 - \left(\frac{\alpha_S\hbar c}{4} R^2\right) \int \Psi_{njlm}^{\mathrm{UA}^+}(\vec{r}_0) \beta \Psi_{njlm}^{\mathrm{UA}}(\vec{r}_0) r_0^{-3} P_2(\cos\theta_0) d\vec{r}_0$$
$$= \frac{[3m^2 - j(j+1)]\lambda^3}{4j(j+1)2\gamma(\gamma^2-1)(4\gamma^2-1)m_0c^2N_0} R^2\hbar c \{\alpha_V[3(N_0^2 - \kappa^2)\alpha_V\hbar c\lambda - 3\kappa m_0c^2(\gamma + n_r) + N_0 m_0c^2(2\gamma^2+1)]$$
$$+ \alpha_S[3(N_0^2 - \kappa^2)\alpha_S\hbar c\lambda + N_0(2\gamma^2+1)E^{\mathrm{UA}} - 3\kappa E^{\mathrm{UA}}(n_r + \gamma)]\}. \tag{14}$$

The formulas (12) and (14) determine the two first terms of the expansion for small R of total energy, which includes the rest energy of the electron of the system,

$$E_{njlm}(\alpha_V,\alpha_S;R)=E^{\mathrm{UA}}+[W^{njlm}_{njlm}]_2+O(R^3). \tag{15}$$

C. Asymptotic behavior of potential curves of two-center problem in separated-atom limit

We shall determine the energy $E(R)$ and the wave function $\Psi(\vec{r};R)$ of the electron in the other limit case, when the distance R between the centers is large. This distance should be so large that the quantum penetrability of the potential barrier, which separates the atomic particles, would be much smaller than a unity. When the constants of the vector α_{V1} and α_{V2} and scalar α_{S1}, α_{S2} coupling are different, the eigenvalues $E(R)$ of the two-center problem are divided into two classes in the asymptotic limit $R\to\infty$: E_{I} and E_{II}—potential curves that for $R\to\infty$ transform into the energy levels of isolated atoms 1 and 2, respectively.

The criterion of applicability of the expansion given below is a requirement that the wave function of the Ψ_1 state, for instance, of atom 1 should not be strongly perturbed by the other particle. The distortion of the dependence of this function on the coordinates should be small. This is related to the energy shift of the state which is induced by the interaction with perturbing particle 2. To be able to apply the perturbation theory, the external field of particle 2 must be weak compared to typical intra-atomic fields.

Similarly to Eq. (8) we represent the complete Hamiltonian of the two-center problem by a Hamiltonian zero approximation $\hat{H}^{\mathrm{SA}}$ and a perturbation $\hat{V}$,

$$\hat{H}=\hat{H}^{\mathrm{SA}}+\hat{V}.$$

Let us introduce the spherical coordinate system $(r_1;\theta_1;\varphi_1)$: its origin is at center 1, and the angle θ_1 is measured from the axis directed from center 1 to center 2. The Hamiltonian of the separated atom 1 will act as $\hat{H}^{\mathrm{SA}}$:

$$\hat{H}^{\mathrm{SA}}=c\vec{\alpha}\cdot\hat{\vec{p}}+\beta\left(m_0c^2-\hbar c\frac{\alpha_{S1}}{r_1}\right)-\hbar c\frac{\alpha_{V1}}{r_1}.$$

At large internuclear distances, the operator of the interaction between the electron and the second center $\hat{V}=-\hbar c\frac{\beta\alpha_{S2}+\alpha_{V2}}{|\vec{r}_1-\vec{R}|}$ can be considered as a small perturbation to the Hamiltonian $\hat{H}^{\mathrm{SA}}$.

The eigenvalues of the operator $\hat{H}^{\mathrm{SA}}$ similarly to $\hat{H}^{\mathrm{UA}}$ are characterized by the set of the quantum numbers n_1, j_1, l_1, and m_1. The eigenfunctions $\Psi^{\mathrm{SA}}_{n_1j_1l_1m_1}(\vec{r}_1)$ are represented by the formulas which are obtained from Eqs. (10) and (11) by substituting $\vec{r}_0\to\vec{r}_1$ and introducing index 1 in the other formulas. The eigenvalues of the operator $\hat{H}^{\mathrm{SA}}$ are determined by the formula (see, for example, [22])

$$E_1=m_0c^2\left\{\frac{-\alpha_{V1}\alpha_{S1}}{\alpha_{V1}^2+(n_1-j_1-1/2+\gamma_1)^2}+\left[\left(\frac{\alpha_{V1}\alpha_{S1}}{\alpha_{V1}^2+(n_1-j_1-1/2+\gamma_1)^2}\right)^2-\frac{\alpha_{S1}^2-(n_1-j_1-1/2+\gamma_1)^2}{\alpha_{V1}^2+(n_1-j_1-1/2+\gamma_1)^2}\right]^{1/2}\right\}.$$

The matrix elements of the operator $\hat{V}$ can be determined from the expansion

$$\hat{V}=-\hbar c(\alpha_{V2}+\beta\alpha_{S2})\left\{\begin{array}{ll}\sum_{s=0}^{\infty}R^s r_1^{-s-1}P_s(\cos\theta_1), & r_1>|\vec{R}|\\ \sum_{s=0}^{\infty}R^{-s-1}r_1^s P_s(\cos\theta_1), & r_1<|\vec{R}|\end{array}\right\}. \tag{16}$$

The matrix $\|V^{n_1j_1l_1'm_1'}_{n_1j_1l_1m_1}\|$, which consists of the following matrix elements,

$$V^{n_1j_1l_1'm_1'}_{n_1j_1l_1m_1}=\int\Psi^{\mathrm{SA}^+}_{n_1j_1l_1m_1}(\vec{r_1})\hat{V}\Psi^{\mathrm{SA}}_{n_1j_1l_1'm_1'}(\vec{r_1})d\vec{r_1},$$

is not diagonal with respect to l_1 (however, it is diagonal with respect to m_1), which is different from the case of the united atom. For the wave functions of the zero-order approximation we can write

$$\Psi_0=\sum_{l_1'm_1'}C^{l_1m_1}_{l_1'm_1'}(R)\Psi^{\mathrm{SA}}_{n_1j_1l_1'm_1'}(\vec{r_1}). \tag{17}$$

By substituting expansion (17) into the Dirac equation with Hamiltonian $\hat{H}$, multiplying by $\Psi^{\mathrm{SA}^+}_{n_1j_1l_1m_1}(\vec{r}_1)$ at the left-hand side, and integrating over the electron coordinates, we achieve the secular equation

$$\sum_{l_1'm_1'}[(E_I-E_1)\delta_{l_1l_1'}\delta_{m_1m_1'}-V^{n_1j_1l_1'm_1'}_{n_1j_1l_1m_1}]C^{l_1m_1}_{l_1'm_1'}(R)=0, \tag{18}$$

where δ_{lm} is the Kronecker δ.

Obviously, the first term in expansion (16) for the perturbation operator is diagonal with respect to mutually degenerated states, the second term contains the following nonzero off-diagonal elements:

$$V^{n_1j_1j_1+1/2m_1}_{n_1j_1j_1+1/2m_1}=V^{n_1j_1j_1-1/2m_1}_{n_1j_1j_1-1/2m_1}=-\frac{\hbar c}{R}\left(\alpha_{V2}+\frac{\alpha_{S2}E_1}{m_0c^2}\right), \tag{19}$$

$$V^{n_1j_1j_1-1/2m_1}_{n_1j_1j_1+1/2m_1}=-V^{n_1j_1j_1+1/2m_1}_{n_1j_1j_1-1/2m_1}=\frac{\hbar c}{R^2}\frac{im_1\sqrt{N_1^2-\kappa_1^2}}{4j_1(j_1+1)\lambda_1m_0c^2N_1}\{\alpha_{V2}[E_1N_1+2m_0c^2(n_{r_1}+\gamma_1)]+\alpha_{S2}[2(n_{r_1}+\gamma_1)E_1+N_1m_0c^2]\}. \tag{20}$$

By using matrix elements (19) and (20) and solving the equation, which is obtained from the condition that the de-

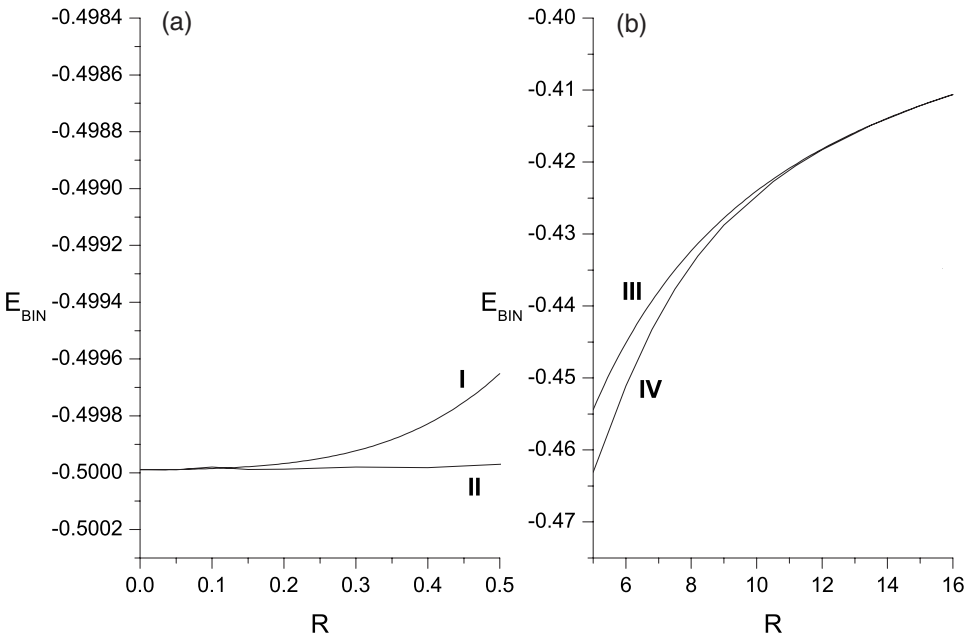

FIG. 3. (a) The ground-state binding energy of the Er^{+68}-Er^{+68} system obtained for $\alpha_S=0.8$ in the united-atom limit: curve I, calculations by asymptotic formula (15); curve II, calculations by the LCAO method (5). (b) The binding energy obtained for $\alpha_S=0.8$ in the separated-atom limit: curve III, calculations by asymptotic formula (21); curve IV, calculations by the LCAO method (5) ($\hbar=m_0=c=1$).

terminant (18) equals zero, we obtain the expression for the energy terms within the first-order perturbation theory,

$$E_I(R) = E_1 - \frac{\hbar c}{R}\left(\alpha_{V2} + \frac{\alpha_{S2}E_1}{m_0c^2}\right) + \frac{\hbar c\Lambda_1}{R^2} + O(R^{-3}),$$

$$\Lambda_1 = \pm \frac{m_1\sqrt{N_1^2-\kappa_1^2}}{4\lambda_1 j_1(j_1+1)N_1 m_0 c^2}\{\alpha_{V2}[E_1N_1 + 2m_0c^2(n_{r_1}+\gamma_1)] + \alpha_{S2}[2E_1(n_{r_1}+\gamma_1) + N_1m_0c^2]\}, \quad (21)$$

where "±" corresponds to the state with $l_1=j_1\pm 1/2$.

The asymptotic expansion of the potential curve E_{II} is obtained from E_I by substituting $E_1\to E_2$, $\alpha_{V1,2}\to\alpha_{V2,1}$; $\alpha_{S1,2}\to\alpha_{S2,1}$; $n_1,\kappa_1,j_1,m_1\to n_2,\kappa_2,j_2,m_2$.

D. Comparing results

It is interesting to compare the results obtained by the variational formula (5) with the results of more precise asymptotic formulas (15) and (21) within the limits of their applicability. As a result, the energy term (5) for the ground state and parameters $R=0.05$, $\alpha_S=0.8$, and $\alpha_V=68/137$ amounts to $2.01\times10^{-4}\%$ of the energy (15). The energy (5) for parameters $R=15$, $\alpha_S=0.8$, and $\alpha_V=68/137$ amounts to $2.7\times10^{-3}\%$ of the energy (21). These comparisons clearly show us a good accuracy of the LCAO method for finding electron binding energy. Dependences of the electron binding energy on R are presented in Fig. 3 for the ground states of the Er^{68+}-Er^{68+} system, which have been calculated by means of the formulas obtained within the LCAO method (5) and the perturbation theory [Eqs. (15) and (21)].

It is important to note that the analytical formulas obtained here for the energy (15) and (21) coincide with the corresponding results of Ref. [8] when $\alpha_S=0$.

III. CRITICAL PHENOMENA

A. Critical charge of nucleus

In Sec. II A we have demonstrated a strong influence of scalar interaction on the electron binding energy (Fig. 2). Therefore, it is natural to expect significant influence α_S on the parameters Z_{cr} and R_{cr} of the theory.

In this section we use the effective-potential method proposed by Popov [38] for obtaining the critical nuclear charge within the model (2) in the limit $L=\ln(1/r_n)\gg1$, when the cutoff radius r_n is arbitrarily small compared to the electron Compton wavelength (so-called logarithmic approximation). Assuming that the potentials of the system are spherical symmetric, we can derive the coupled radial differential equations in the usual way [22] (in this section the relativistic units $\hbar=m_0=c=1$ are used):

$$\frac{dF}{dr} = -\frac{\kappa}{r}F + [\varepsilon + 1 + \hat{S}(r) - \hat{V}(r)]G,$$

$$\frac{dG}{dr} = \frac{\kappa}{r}G - [\varepsilon - 1 - \hat{S}(r) - \hat{V}(r)]F, \quad (22)$$

where

$$F(r) = rf(r), \quad G(r) = rg(r),$$

and $\varepsilon=E/m_0c^2$ is the electron energy.

We consider the region $r\sim0$, where the constant terms proportional to the mass and energy can be neglected. Using the transformation

$$\begin{Bmatrix} F \\ G \end{Bmatrix} = \Phi_i(r)\sqrt{V\mp S}, \quad i=1,2,$$

we can reduce Eq. (22) to the form of a self-adjoint Shrödinger equation

$$\Phi_i'' + k_i^2(r)\Phi_i = 0, \tag{23}$$

where

$$k_i^2(r) \overset{r\to 0}{=} V^2 - S^2 + \frac{(V \mp S)''}{2(V \mp S)} - \frac{3}{4}\frac{[(V \mp S)']^2}{(V \mp S)^2} \mp \frac{\kappa}{r}\frac{(V \mp S)'}{(V \mp S)} \mp \frac{\kappa(\pm\kappa + 1)}{r^2}.$$

Let potentials $\hat{S}(r)$ and $\hat{V}(r)$ have the form (2) at small r; thus

$$k_i^2(r) \simeq \frac{\alpha_V^2 - \alpha_S^2 - j(j+1)}{r^2}.$$

The form of the wave function can be obtained from (23) at small distances r,

$$\Phi(r) \sim r^\sigma, \quad \sigma_{1,2} = \tfrac{1}{2} \pm \gamma, \quad \gamma = \sqrt{\kappa^2 - \alpha_V^2 + \alpha_S^2}.$$

Let us first suppose that $\alpha_V^2 - \alpha_S^2 < \kappa^2$; hence, σ_1 and σ_2 are real and $\sigma_1 > \sigma_2$. Thus, from two solutions, we must choose one which becomes infinite less rapidly. Next, let $\alpha_V^2 - \alpha_S^2 > \kappa^2$; therefore, $\sigma_{1,2} = \frac{1}{2} \pm i\gamma$ are complex, and both solutions have the form

$$\Phi(r) \overset{r\to 0}{=} \sqrt{r}\sin(g \ln r + \text{const}), \quad g = i\gamma = \sqrt{\alpha_V^2 - \alpha_S^2 - \kappa^2}. \tag{24}$$

The presence of oscillating asymptotics (24) indicates that the level with $\varepsilon = -1$ exists. Therefore, using the terminology from [38], we will call the value $|\alpha_{V\,\mathrm{cr}}^p| = \sqrt{\kappa^2 + \alpha_S^2}$ as a "critical charge" of a pointlike nucleus. At $\alpha_S \to 0$ we reach $Z_{\mathrm{cr}}^p = 137\alpha_{V\,\mathrm{cr}}^p = 137(j + 1/2)$, which coincides with the results from [38].

Now we will demonstrate how to find $\alpha_{V\,\mathrm{cr}}$ in the cutoff potential. For simplicity, we will consider the case when $r_n \ll \lambda_c = \hbar/m_0c^2$ [more exactly $L = \ln(1/r_n) \gg 1$]. On the one hand, the wave function in the region $r_n < r \ll 1$ has the form (24). On the other hand, the ground-state wave function $\Phi_0(r)$ cannot have zeros; wherefrom

$$gL < \pi.$$

The maximum of the value $g = g_{\mathrm{cr}} = \pi/L$ corresponds to the moment when the lowest level with this j has reached $\varepsilon = -1$ [in the case $g > g_{\mathrm{cr}}$, $\Phi(r)$ would have a zero, which is impossible]. From the condition $g_{\mathrm{cr}} = \pi/L$, we find that

$$|\alpha_{V\,\mathrm{cr}}| = |Z_{\mathrm{cr}}\alpha| = \sqrt{\kappa^2 + \alpha_S^2 + \left(\frac{\pi}{L}\right)^2}. \tag{25}$$

Therefore, the following asymptotic formula can be obtained:

$$|\alpha_{V\,\mathrm{cr}}| = \sqrt{\kappa^2 + \alpha_S^2}\left(1 + \frac{\pi^2}{2(\kappa^2 + \alpha_S^2)L^2}\right) + O(L^{-3}).$$

The first term of this expansion defines the value of the critical charge of the pointlike nucleus, and the second term takes into account a finite size of the nucleus. At $\alpha_S \to 0$ this formula coincides with the result by Popov [38]. In the same work, it has been shown that this approach has a good accuracy even at $r_n = 10^{-12}$ cm, $L = 3.5$. Equation (25) is transcendental with respect to $\alpha_{V\,\mathrm{cr}}$. To solve it, we accept that $r_n = r_0 A^{1/3}$, where $r_0 = 1.1$ fm and the dependence of A on the charge of the nucleus is defined by the formula $A = 2.6Z$ following [40] (see curve II in Fig. 5). The solution of Eq. (25) for different values α_S is given in Fig. 4. In accordance with Eq. (25), we observe that the critical charge Z_{cr} increases with increasing the scalar coupling constant α_S.

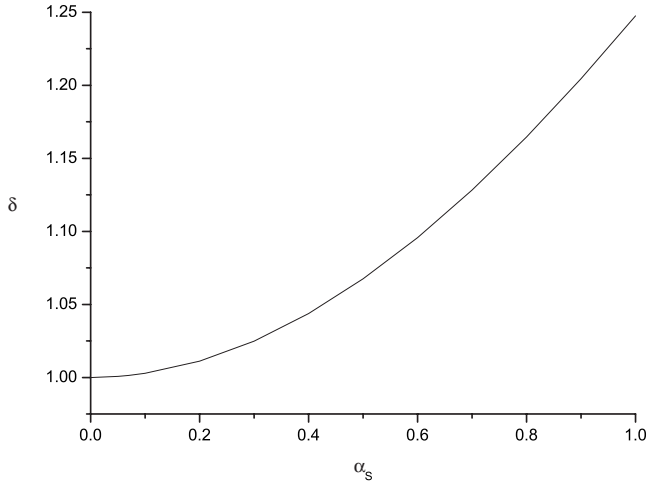

FIG. 4. The dependence of the ratio $\delta = (Z_{\mathrm{cr}})_{S+V}/(Z_{\mathrm{cr}})_V$ on the scalar coupling constant α_S, where $(Z_{\mathrm{cr}})_{S+V}$ $[(Z_{\mathrm{cr}})_V]$ is the critical charge which takes into account (neglects) the scalar interaction.

The formula (25) at $\alpha_S = 0$ gives the value $Z_{\mathrm{cr}} = 185$ (which exceeds the exact value $Z_{\mathrm{cr}} \approx 170$), so the obtained formulas can be used only for the qualitative description of the dependence of the critical charge Z_{cr} on α_S. Better results can be obtained within the more strict investigation of the Dirac equation with potentials (2) [43].

B. Critical distance for colliding nuclei

In this section we investigate the influence of scalar coupling constant α_S on the value of critical distance R_{cr} in collisions of heavy ions. The critical distance R_{cr} is the maximal separation between the heavy ions at which spontaneous positron production may occur. For this purpose we use a method of matching the asymptotics proposed in [41]. The configuration space in the two-center problem can be divided into three regions: $r_1 \ll R$ or $r_2 \ll R$ (region I); $r_1, r_2 \gg R$ (region II); r_1 and $r_2 \sim R$ (region III). We shall find the solution of the Dirac equation in region I and region II (Ψ_{I} and Ψ_{II} accordingly). In Ref. [42] it was shown that the solutions Ψ_{I} and Ψ_{II} must be sewn under the condition $\varepsilon = -1$. For this purpose it is necessary to consider the behavior of Ψ_{I} and Ψ_{II} in intermediate region III.

Let us investigate the wave function Ψ at $\varepsilon = -1$ near to nuclei (region I). For this purpose we shall write the Dirac equation in the following form:

$$(\vec{\sigma}\cdot\hat{\vec{p}})\varphi = -[\hat{V}(\vec{r}) - \hat{S}(\vec{r})]\chi,$$

$$(\vec{\sigma}\cdot\hat{\vec{p}})\chi = -[\hat{V}(\vec{r}) + \hat{S}(\vec{r}) + 2]\varphi, \tag{26}$$

where φ and χ are upper and lower bispinor components, respectively. The substitution $\Phi = (\hat{V}-\hat{S})^{-1/2}\varphi$ transforms these equations into one which is similar to the Schrödinger equation with an effective potential $\hat{U}$,

$$(\Delta - 2\hat{U})\Phi = 0, \tag{27}$$

where

$$\hat{U} = -\hat{V} + \hat{S} + \frac{\hat{S}^2 - \hat{V}^2}{2} + \frac{\Delta(\hat{V}-\hat{S})}{4(\hat{V}-\hat{S})} + \frac{3}{8}\left(\frac{\vec{\nabla}(\hat{V}-\hat{S})}{\hat{V}-\hat{S}}\right)^2 - \frac{\vec{\sigma}[\vec{\nabla}(\hat{V}-\hat{S}),\hat{\vec{p}}]}{2(\hat{V}-\hat{S})}.$$

It is convenient to investigate Eq. (27) using the elliptic coordinates $(\xi;\ \eta;\ \varphi)$. The wave function near to the nuclei has the following form [42]:

$$\Phi(\xi,\eta) \sim (\xi^2 - \eta^2)^{\rho}. \tag{28}$$

Inserting Eq. (28) into Eq. (27) and taking into account only terms $\sim R^{-2}$ $(R \ll 1)$, we obtain

$$\rho = -\tfrac{1}{2} \pm \gamma, \quad \gamma = \sqrt{1 - \alpha_V^2 + \alpha_S^2}.$$

Thus, near the nuclei

$$\varphi_{\mathrm{I}}, \chi_{\mathrm{I}} \sim (\xi^2 - \eta^2)^{\gamma - 1}$$

(from two solutions we must choose one which becomes infinite less rapidly). We can obtain the wave function in exterior region II from the Dirac equation with the potential

$$\hat{V} + \beta\hat{S} = -\frac{\zeta_V}{r} - \beta\frac{\zeta_S}{r} \quad (\zeta_{V,S} = 2\alpha_{V,S}).$$

The equations for the radial functions of the ground state have the following form at $r \ll 1$:

$$\frac{dF}{dr} = \frac{F}{r} + \frac{\zeta_V - \zeta_S}{r}G,$$

$$\frac{dG}{dr} = -\frac{G}{r} - \frac{\zeta_V + \zeta_S}{r}F. \tag{29}$$

Solving this system, we will obtain

$$F = \sin\left(\beta - g_2 \ln\frac{2r}{R}\right), \quad G = -\sin\left(\tilde{\beta} - g_2 \ln\frac{2r}{R}\right),$$

where

$$\tilde{\beta} - \beta = \arctan g_1, \quad g_1 = \sqrt{(\zeta_V - \zeta_S)^2 - 1}, \quad g_2 = \sqrt{\zeta_V^2 - \zeta_S^2 - 1}.$$

By comparing our result with the exact solution of the Dirac equation, we have defined the phase $\beta = \arg\Gamma(1+2ig_2) - g_2 \ln[(\zeta_V - \zeta_S)R]$.

It is easy to show that at $R \ll r \ll 1$,

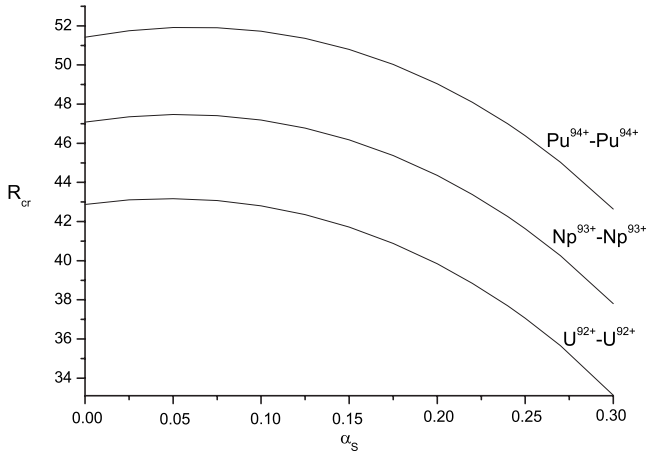

FIG. 5. The dependence of the critical distance R_{cr} (fm) on the scalar coupling constant α_S for three different systems of colliding heavy nuclei.

$$\varphi_{\mathrm{II}} \sim \xi^{-(1+g_2\cot\beta)}, \quad \chi_{\mathrm{II}} \sim \xi^{-(1+g_2\cot\tilde{\beta})}.$$

After matching the probability-distribution density $\rho = \Psi^{\dagger}\Psi$, which is integrated over the spinor indexes, in region III $R \ll r \ll 1$ (for details see [42]), we obtain the formula for R_{cr},

$$R_{\mathrm{cr}} = \frac{1}{2(\alpha_V - \alpha_S)}\exp\left[-\frac{1}{g_2}\left(\frac{\pi}{2} - \arctan\tilde{\eta} - \arg\Gamma(1+2ig_2)\right)\right], \tag{30}$$

here

$$\tilde{\eta} = \frac{(1-2\gamma)g_1 + (\zeta_V - \zeta_S - 1)g_2}{g_2 g_1 + (2\gamma - 1)(\zeta_V - \zeta_S - 1)}.$$

Expression (30) at $\alpha_S = 0$ coincides with the well-known Popov formula (11) [42].

The results obtained by means of formula (30) for the ground states of three different systems of colliding heavy nuclei U^{92+}-U^{92+}, Np^{93+}-Np^{93+}, Pu^{94+}-Pu^{94+} are shown in Fig. 5. From this figure it is clear that the function R_{cr} has maximum at $\alpha_S \sim 0.06-0.08$ and afterwards monotonously falls down with increasing α_S.

In the end of the paper we would like to check an accuracy of the method of matching the asymptotics. For this purpose we have considered the problem of the critical charge of the nucleus within the model (2) and have checked the formula obtained with the exact results of work [43]. Thus, the following formula was obtained for the critical charge $\alpha_{V\,\mathrm{cr}}$ of a spherical nucleus with the radius r_n,

$$r_n = \frac{1}{2(\alpha_{V\,\mathrm{cr}} - \alpha_S)}\exp\left\{-\frac{1}{g_0}\left[\frac{\pi}{2} - \arctan\left(-\frac{\zeta}{g_0}\right) - \arg\Gamma(1+2g_0)\right]\right\}, \tag{31}$$

where

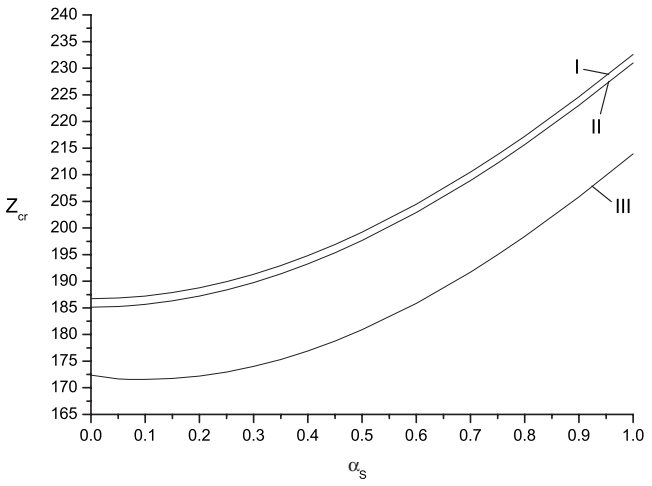

FIG. 6. The dependence of the critical charge value Z_{cr} on the scalar coupling constant α_S. Curve I is obtained by solving Eq. (25) with the assumptions $r_0=1.2$ fm and $A=63.6+1.3Z+0.007\,33Z^2$ [39]. Curves II and III are obtained by formulas (25) and (31) with the assumptions $r_0=1.1$ fm and $A=2.6Z$.

$$g_0=\sqrt{\alpha_{V\,\mathrm{cr}}^2-\alpha_S^2-1},\quad \zeta=\left.(rF'/F)\right|_{r=r_n}.$$

Equation (31) is transcendental with respect to $\alpha_{V\,\mathrm{cr}}=Z_{\mathrm{cr}}\alpha$. The numerical solution of Eq. (31) is shown in Fig. 6 (curve III). The function $Z_{\mathrm{cr}}(\alpha_S)$ has a minimum at $\alpha_S\sim 0.08-0.1$ and grows dramatically with increasing α_S. The comparison of expression (31) with the results of the exact calculations [see Eq. (45) in [43]] reveals that this formula provides Z_{cr} to a percent precision. Expression (31) at $\alpha_S=0$ coincides with the Popov formula (11) [42].

It is necessary to note that following [43] we used the rectangular cutoff model of the potentials (2). The logarithmic derivative can be found analytically (for the ground state) within this simple model

$$\zeta=\sqrt{\alpha_{V\,\mathrm{cr}}^2-\alpha_S^2}\,\cot\sqrt{\alpha_{V\,\mathrm{cr}}^2-\alpha_S^2}.$$

IV. CONCLUSIONS

In this paper we investigate the two-center problem for the Dirac equation with a Coulomb and scalar potential. By means of the LCAO method, we calculate the ground-state wave function and the energy term of the electron as functions of the internuclear distance R and the coupling constants α_V and α_S. The expressions for the energy in the united-atom and separated-atom limits are obtained for arbitrary states of the two-center system by means of the perturbation theory. The obtained analytic results show that the energy increases with increasing the value α_S. Apart from the fundamental results obtained for the two-center problem, we investigate the dependence of the critical charge Z_{cr} and the critical distance R_{cr} on α_S. A strong influence of the Lorentz structure of the interaction potentials on the critical charge and the critical distance is revealed.

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