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Variational Approach to the Relativistic Two-Center Problem: Critical Internuclear Distance

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As shown recently, if the distance between two heavy nuclei becomes less than its critical value, R_{cr}, their electric potential is strong enough to create electron-positron pairs from the vacuum. This process may occur when the ground level of the quasimolecule (Z, Z, e) is lower than $-m_e c^2$. In order to find R_{cr} the Dirac equation with two Coulomb centers is considered. By means of a proper choice of coordinates and using the variational principle the problem is reduced to a set of ordinary linear differential equations with singular coefficients. To solve the boundary problem the Riccati equation for the logarithmic derivative matrix was considered. The computations are carried out and R_{cr} is found as a function of the nuclear charges. By virtue of the variational principle the obtained quantity is a sure *lower* limit for R_{cr}.

I. INTRODUCTION

Spontaneous creation of electron-positron pairs in superstrong electrostatic potentials is of considerable interest for the quantum electrodynamics as a test of the Dirac equation and of some fundamental properties of the physical vacuum. The potential wells, deep enough to produce such an effect, may be realized in collisions of heavy ions with a supercritical total charge $Z_1 + Z_2 > Z_{cr} \approx 170$. Such an experiment is reported to be in plans at some laboratories and, probably, will be set up in a not too remote future. The theory of this effect was substantially advanced in a number of recent works [1–8]. Of great importance is an accurate calculation of the quantity, the principal for the effect, of the critical internuclear distance R_{cr}, i.e., the maximal distance necessary for the pair creation. In other words, R_{cr} is the value of the internuclear distance R at which the ground term of the quasimolecule (Z_1, Z_2, e^-) crosses the boundary of the lower continuum, the electron energy being $\epsilon = -mc^2$. The spontaneous creation of positrons occurs while the vacant level with $\epsilon < -mc^2$ is occupied by an electron from the vacuum. To know the accurate value of R_{cr} is very important because (as shown in Refs. [4, 5]) the total cross section depends sharply on R_{cr}, $\sigma \sim R_{cr}^{7/2}$; besides, the threshold energy of the heavy ion beam is determined by R_{cr}.

In order to calculate R_{cr}, one needs to solve the eigenvalue problem for the Dirac equation with the potential of two Coulomb centers. Contrary to the non-relativistic case, the variables cannot be separated and the problem is essentially two-dimensional. The subject of the present work is a variational approach reducing the problem to a set of ordinary differential equations that may easily be solved by a computer. The idea of solving the boundary problem for partial differential equations by reducing it to ordinary equations is well known as the Kantorovich method (see its description in [9]). Its application to the Dirac equation is presented in Section II. The resulting linear differential equations are considered in Section III. They were solved using the method elaborated by Abramov *et al.* [10]. The results on R_{cr} are presented and discussed in Section IV. Results concerning the model problem of the scalar particle in the two-center potential are also presented there. Explicit formulas for the coefficient functions are presented in the Appendix.

The R dependence of electron energy levels in a molecule consisting of two heavy atoms may also be of interest (cf. Ref. [11]). We did not extend our calculations to this case; however, the method is applicable and some necessary formulas are given in Section II.

As a rule, we use the natural units: $\hbar = c = m_e = 1$; $\alpha = e^2 = 1/137$, $\zeta = 2Z\alpha$.

II. The Variational Approach

2.1. *Primary Equations*

The bound state problem for the relativistic electron in a potential $V(\mathbf{r})$ is equivalent to searching for the extremum of the functional

$$J = \int \Psi^*(-i\boldsymbol{\alpha}\nabla + \beta m + V - \epsilon)\Psi \, d^3r \tag{2.1}$$

in the space of the four-component bispinor functions $\Psi(\mathbf{r})$ with the norm

$$N = \int \Psi^*\Psi \, d^3r. \tag{2.2}$$

To reduce the number of unknown functions, exclude two lower components of Ψ using the Dirac equation explicitly. Note that no approximate reduction of the Dirac bispinors was used to obtain Eqs. (2.3)–(2.6). Then for the spinor ξ formed by the upper components of Ψ we get

$$J = \int [(m + \epsilon - V)^{-1} |(\boldsymbol{\sigma}\nabla)\xi|^2 + (m - \epsilon + V)|\xi|^2] \, d^3r, \tag{2.3}$$

$$N = \int [(m + \epsilon - V)^{-2} |(\boldsymbol{\sigma}\nabla)\xi|^2 + |\xi|^2] \, d^3r. \tag{2.4}$$

The functional J may be represented in a form specific for the non-relativistic quantum mechanics [12, 13] introducing another spinor field $\psi = (m + \epsilon - V)^{-1/2}\,\xi$,

$$J = \int [|\,\nabla\psi\,|^2 + i(\nabla\psi^*)(\mathbf{F}\times\sigma)\psi - i\psi^*(\mathbf{F}\times\sigma)\,\nabla\psi + 2(U-E)\,|\,\psi\,|^2]\,d^3r, \quad (2.5)$$

where

$$\mathbf{F} = -\tfrac{1}{2}(m+\epsilon-V)^{-1}\,\nabla V, \quad U = \epsilon V - \tfrac{1}{2}V^2 + \tfrac{1}{2}(\mathbf{F}^2 - \nabla\mathbf{F}), \quad E = \tfrac{1}{2}(\epsilon^2 - m^2);$$

E is the effective energy, U is the effective scalar potential (depending on the energy), the spin–orbit coupling with field $\mathbf{F}$ is also present. Note that the norm in space of the ψ functions is somewhat unconventional.

$$N = \int [|\,\nabla\psi\,|^2 + i(\nabla\psi^*)(\mathbf{F}\times\sigma)\psi - i\psi^*(\mathbf{F}\times\sigma)\,\nabla\psi + W]\,\tilde{V}^{-1}\,d^3r, \quad (2.6)$$

where

$$\tilde{V} = m + \epsilon - V; \qquad W = \tilde{V}^2 - (\mathbf{F}^2 + \nabla\mathbf{F}).$$

This norm does not affect the equation obtainable from (2.5); however, it is important for boundary conditions.

The matter of interest for us now is to find a potential V for which the energy level crosses the boundary of the lower continuum. So, put $\epsilon = -m$ (the functional is then much simplified); the resulting equation for ψ is the Schrödinger equation with an effective potential and zero energy. This approach was very useful in finding the critical charge (assuming for V the Coulomb form with a cutoff at $r < r_N$; the discussion is given in Ref. [2]), as well as in a qualitative analysis of the problem in view [12, 14].

Consider the potential of two identical pointlike charges Ze,

$$V = -\tfrac{1}{2}\zeta(r_1^{-1} + r_2^{-1}), \qquad \zeta = 2Z\alpha, \quad (2.7)$$

where r_1 and r_2 are distances to the centers. It may be shown that in the relativistic case the variables cannot be separated and with account of the axial symmetry the problem is essentially two-dimensional. Introduce the cylindrical coordinates (ρ, z, φ) with the origin halfway between the centers; $r_{1,2} = [\rho^2 + (z \mp R/2)^2]^{1/2}$. The ground state has the total angular momentum projection $M_Z = \frac{1}{2}$; the projection of the orbital momentum Λ is 0 for the upper component ($\psi_\uparrow$) and 1 for the lower component ($\psi_\downarrow$). The ground state has the positive parity with respect to reflection in the plane $z = 0$. This implies that $\psi_\uparrow$ is an even function of z while $\psi_\downarrow$ is odd. Besides, due to the centrifugal barrier, $\psi_\downarrow$ must have a simple zero

at $\rho = 0$. With all this in view one may write

$$\psi_\uparrow(\mathbf{r}) = \chi_1(\rho, z), \qquad \psi_\downarrow(\mathbf{r}) = 4R^{-2}\rho z \exp(i\varphi)\, \chi_2(\rho, z), \tag{2.8}$$

where $\chi_{1,2}$ are real functions of two variables, even in z and with no kinematical zeros. Substituting (2.8) into Eq. (2.5) and integrating over φ one gets

$$J = \int_0^\infty \rho\, d\rho \int_0^\infty dz\{\tfrac{1}{2}(\partial\chi_1)^2 + \tfrac{1}{2}(\partial\beta\chi_2)^2 + U_{11}\chi_1{}^2 + 2\beta U_{12}\chi_1\chi_2 + \beta^2 U_{22}\chi_2{}^2 + \chi_1\hat{\Lambda}\beta\chi_2 - \beta\chi_2\hat{\Lambda}\chi_1\}, \tag{2.9}$$

where

$$(\partial\chi)^2 = (\partial\chi/\partial\rho)^2 + (\partial\chi/\partial z)^2, \qquad \beta = 4R^{-2}\rho z,$$
$$U_{11} = -V - \tfrac{1}{2}V^2 + \tfrac{3}{2}\mathbf{F}^2, \qquad U_{12} = \rho^{-1}F_z\,,$$
$$U_{22} = U_{11} + \rho^{-1}F_\rho + \tfrac{1}{2}\rho^{-2}, \qquad \hat{\Lambda} = F_z\,\partial/\partial\rho - F_\rho\,\partial/\partial z,$$
$$F_\rho = \tfrac{1}{2}V^{-1}\,\partial V/\partial\rho, \qquad F_z = \tfrac{1}{2}V^{-1}\,\partial V/\partial z.$$

2.2. *Test Functions*

The idea of the present approach is as follows. Introduce new variables

$$x = X(\rho, z), \qquad y = Y(\rho, z). \tag{2.10}$$

In the separable case the choice of (x, y) is evident; there is a solution independent on y; e.g., for a potential with spherical symmetry we would like $x = (\rho^2 + z^2)^{1/2}$, $y = \rho/z$. There is no separable system in our case, so we prefer such coordinates that the solution has singularities in x, while there is no singularity in y. Such a system may be called asymptotically separable. The singularities of our problem locate at $r_1 \to 0$, $r_2 \to 0$, and at infinity. So the function X in (2.10) is to be chosen in such a way that $x \to 0$ at $r_1 \to 0$ or $r_2 \to 0$, and $x \gg 1$ at $r_1\,, r_2 \gg R$. Besides, it is appropriate to use functions even in z (i.e., pertaining to the symmetry $r_1 \leftrightarrow r_2$).

With such new variables substitute the unknown functions in the functional J by finite sums:

$$\chi_1 = \sum_{k=1}^{m} \varphi_k(x)\, y^{k-1}, \qquad \chi_2 = \sum_{k=1}^{n} \varphi_{m+k}(x)\, y^{k-1}, \tag{2.11}$$

where φ_k $(k = 1,..., N = m + n)$ are arbitrary functions of x. Minimization of the functional on this class of test functions is called the (m, n)-approximation.

Integrating over y we get the functional in the form

$$J = \int \sum_{k,l} (P_{kl}\varphi_k'\varphi_l' + Q_{kl}\varphi_k\varphi_l + 2R_{kl}\varphi_k'\varphi_l)\, dx, \tag{2.12}$$

where **P**, **Q**, **R** are matrices depending on x. An analogous formula may be obtained for the norm. Minimization of (2.12) leads to a set of linear second-order differential equations for functions φ_k with boundary conditions resulting from integrability of the norm. This problem is much simpler than the primary pair of partial differential equations and is discussed in the next section. If asymptotically separable coordinates are chosen the correct singularities occur in the test functions enabling one to obtain good accuracy. Note, for instance, that in elliptic coordinates, $x = (r_1 + r_2)/R$, $y = (r_1 - r_2)/R$, the singularity at $r_{1,2} \to 0$ is not separable ($x \to 1$, $y^2 \to 1$). The resulting values of R_{cr} were far from accurate (calculations in [15]).

Two asymptotically separable coordinate systems were tried. In one of them the curves $x = \text{const}$ are the equipotentials

$$x = 2R^{-1}r_1r_2/(r_1 + r_2), \qquad y = (r_1 - r_2)^2/(r_1 + r_2)^2. \tag{2.13}$$

In the other the curves $x = \text{const}$ are the Cassinian ovals

$$x = 4R^{-2}r_1r_2\,, \qquad y = (r_1 - r_2)^2/4r_1r_2\,. \tag{2.14}$$

Both the variants have some similar properties: (i) the region of x is $(0, \infty)$ with singularities at boundaries, (ii) the region of y at fixed x is $(y_1(x), y_2(x))$ where the derivative of y_1 is discontinuous at $x = 1$ due to a change of topology of the surface $X(\rho, z) = x$. The calculation shows that both the systems result in very close values of R_{cr}, while the latter is better (the curve $R_{cr}(Z)$ is somewhat higher). So the subject of the subsequent discussion will be the Cassinian choice (2.14).

In our approach the leading singularities in the test functions are those of the exact solution, analyzed in detail previously [14]. At small x (near a nucleus) the power singularity arises from the term $\sim r^{-2}$ in the effective potential (V^2 in Eq. (2.9)):

$$\chi(x, y) \sim x^{-\sigma}, \qquad \sigma = 1 - (1 - \zeta^2/4)^{1/2}. \tag{2.15}$$

Note that for $Z < 137$ ($\zeta < 2$) there is no "collapse" in the nuclear field, so it is not necessary to cut off the potential at small r and the nuclei may be considered as pointlike. At large x the singularity is determined by the repulsive Coulomb tail ($-V$ in Eq. (2.9)):

$$\chi(x, y) \sim \exp[-2(\zeta R)^{1/2}\, x^{1/4}]. \tag{2.16}$$

Consider now the integration over the inessential variable y.

2.3. *Reduction to One-Dimensional Problem*

Substituting the test functions (2.11) into Eq. (2.9) with variables (2.14), one gets

$$J = \int_0^\infty dx \int_{y_1}^{y_2} dy\, D(x, y) \sum_{i,j} (p_{ij}\varphi_i'\varphi_j' + q_{ij}\varphi_i\varphi_j + 2r_{ij}\varphi_i'\varphi_j), \tag{2.17}$$

where

$$y_2(x) = x^{-1}, \qquad y_1(x) = x^{-1} - 1 \quad \text{at} \quad x \leqslant 1, \quad y_1(x) = 0 \quad \text{at} \quad x > 1; \tag{2.18}$$

$D(x, y)$ is the Jacobian

$$D(x, y) = \rho \frac{\partial(\rho, z)}{\partial(x, y)} = \frac{1}{16} R^3 x[y(y+1)]^{-1/2}, \tag{2.19}$$

and p_{ij}, q_{ij}, r_{ij} are some functions of x and y (see the Appendix). Integration over y results in the functional (2.12) with the x-dependent matrices:

$$P_{ij}(x) = \int_{y_1}^{y_2} p_{ij}(x, y)\, D(x, y)\, dy, \tag{2.20}$$

etc., given explicitly in the Appendix.

In general, the coefficient matrices **P**, **Q**, **R** depend on the choice of the second variable y. With our choice we succeeded in expressing all the matrix elements in terms of elementary functions. However, the matrices **P**, **Q**, **R** are simultaneously degenerating near singularities. For instance, at $x \to 0$ and $m = 2$, $n = 1$,

$$\begin{aligned} &P_{11} = \tfrac{1}{2}x^2 + O(x^4), && P_{12} = P_{21} = \tfrac{1}{2}x(1 - \tfrac{1}{2}x) + O(x^3), \\ &P_{22} = \tfrac{1}{2}(1 - x) + O(x^2), && P_{33} = (1/12)\, x^4 + O(x^5), \\ &P_{13} = P_{23} = P_{31} = P_{32} = 0, \end{aligned} \tag{2.21}$$

while $\det \mathbf{P} = O(x^8)$. Dealing with the resulting set of ordinary differential equations one has to analyze the asymptotics of the matrices and to exclude some inessential singularities.

III. Boundary Problem for Ordinary Differential Equations

3.1. *Riccati Matrix Equation*

Minimization of the functional (2.12) leads to the set of linear differential equations (in this section we use the matrix notations):

$$\frac{d}{dx}\left(\mathbf{P}\frac{d\varphi}{dx} + \mathbf{R}\varphi\right) - \mathbf{Q}\varphi - \mathbf{R}^T\frac{d\varphi}{dx} = 0, \tag{3.1}$$

$0 < x < \infty$, with the boundary condition resulting from convergence of the normalization integral.

In order to find the eigenvalues the absolute normalization of φ is of no importance. Consider a matrix $\mathbf{Y}$,

$$\varphi' = \mathbf{Y}\varphi. \tag{3.2}$$

The system (3.1) is satisfied if $\mathbf{Y}$ is a solution of the Riccati matrix equation

$$\mathbf{Y}' = \mathbf{A} + \mathbf{B}\mathbf{Y} - \mathbf{Y}^2, \tag{3.3}$$

where

$$\mathbf{A} = \mathbf{P}^{-1}(\mathbf{Q} - \mathbf{R}'), \qquad \mathbf{B} = -\mathbf{P}^{-1}(\mathbf{R} - \mathbf{R}^T + \mathbf{P}'). \tag{3.4}$$

As for the boundary conditions, the situation is somewhat less trivial. In our case the matrices $\mathbf{A}$ and $\mathbf{B}$ are singular at the boundaries. To obtain a reasonable boundary condition to supplement Eq. (3.3), assume that near a singular point ($x = 0$) $\mathbf{Y}$ has the form

$$\mathbf{Y} = x^{-\nu}(\mathbf{Y}_1 + x\mathbf{Y}_2 + \cdots). \tag{3.5}$$

The exponent ν, as well as the constant matrices $\mathbf{Y}_k$, is to be found from Eq. (3.3). In case of the regular singularity in the system (3.1), $\nu = 1$. Expanding $\mathbf{A}$ and $\mathbf{B}$ near the singular point one gets a sequence of linear recursive equations for $\mathbf{Y}_2$, $\mathbf{Y}_3$,...; the first equation for $\mathbf{Y}_1$ is, however, quadratic,

$$\mathbf{Y}_1^2 - \mathbf{B}_1\mathbf{Y}_1 - \mathbf{A}_1 = 0, \tag{3.6}$$

with some matrix coefficients $\mathbf{A}_1$ and $\mathbf{B}_1$. To select the necessary solution of this equation among the infinite set of matrices satisfying it, one must look at φ near the singularity, finding it from Eq. (3.3) and the initial boundary condition for φ. Fortunately, in our case the selection is straightforward and corresponds to the choice of the less singular test functions (details in Section 3.2).

The proposed procedure is as follows. Take a small x_0 and a large x_∞. Find the expansion (3.5) and its analog at $x \gg 1$, the number of terms being determined by the necessary accuracy. Starting from these points with the initial values given by the expansions and solving the differential equation (3.3), obtain the left and right limits of $\mathbf{Y}$ at an intermediate point x_1 (we use $x_1 = 1$), $\mathbf{Y}^{(0)}(x_1)$ and $\mathbf{Y}^{(\infty)}(x_1)$. The problem is solved if φ and φ' are continuous at x_1. Thus, it is necessary that

$$\Delta(\zeta, R_{cr}) = \det[\mathbf{Y}^{(0)}(x_1) - \mathbf{Y}^{(\infty)}(x_1)] = 0. \tag{3.7}$$

In general, to find the eigenvalue (in our case to find $R = R_{cr}$ at fixed ζ) one has to solve the algebraic equation (3.7). If one considers the extremal eigenvalue (the maximal R_{cr}) the eigenfunctions are nonzero and $\mathbf{Y}$ is nonsingular inside the interval. Taking the correct branches near the singular points from the very beginning, it is possible to get rid of unpleasant oscillations of $\mathbf{Y}$, inevitable in another approach.

After the eigenvalue is found one may wish to obtain the variational test functions. Then one may proceed as follows. The degenerate matrix $\mathbf{D} = \mathbf{Y}^{(0)}(x_1) - \mathbf{Y}^{(\infty)}(x_1)$ is known. Diagonalize it, $\mathbf{D} = \mathbf{C}^{-1}\hat{\mathbf{D}}\mathbf{C}$, $\hat{\mathbf{D}} = \mathrm{diag}(0, d_2, \ldots)$ (one of the eigenvalues of $\mathbf{D}$ is zero!). Now solve the combination of the equations (3.2) and (3.3) in the inverse direction (i.e., from x_1 to x_0 and to x_∞), while the initial value of φ may be taken in form $\varphi(x_1) = \mathbf{C}\hat{\varphi}$ where $\hat{\varphi}_1 = 1$, $\hat{\varphi}_k = 0$ for $k \neq 1$. The resultant $\varphi(x_0)$ provides one with the initial value for an analytical solution of Eq. (3.2) with $\mathbf{Y}$ in the form of Eq. (3.5). The asymptotics of $\varphi(x)$ near $x = \infty$ is obtained in the same way starting from $\varphi(x_\infty)$. The normalization integral is easily calculated in parallel with $\varphi(x)$ and $\mathbf{Y}(x)$.

The formal reason for singularity in Eq. (3.3) at $x = 0$ is that $\det \mathbf{P}$ vanishes (see Eq. (2.22)). However, some matrix elements of $\mathbf{Q}$ and $\mathbf{R}$ also vanish at $x \to 0$. In order to evaluate the indeterminate form and to deal with moderate numbers we transform the coefficients (3.4). The region of large x is in the same situation. Besides, it is useful to map the interval $(1, \infty)$ on the interval $(0, 1)$, so that both parts of our process are as similar as possible. This is the subject of the next section.

3.2. *Transformation of the Riccati Equation*

(a) *General formulas.* Because the matrices $\mathbf{P}$, $\mathbf{Q}$, $\mathbf{R}$ become degenerate at the singularities, as was noted in Section 2.3, various $\varphi_k(x)$, as well as elements of the matrix $\mathbf{Y}(x)$, have quite different orders of magnitude near the singularities. This is rather inconvenient for computations. To cure this difficulty, consider a linear transformation of the test functions

$$\varphi = \mathbf{S}(x)\,\varphi_S\,, \qquad \det \mathbf{S}(x) \neq 0. \tag{3.8}$$

For the transformed matrix $\mathbf{Y}_S(x)$, $\varphi_S' = \mathbf{Y}_S\varphi_S$, we get the same Riccati equation (3.3) with new coefficients $\mathbf{A}_S$ and $\mathbf{B}_S$:

$$\begin{aligned} \mathbf{Y}_S &= \mathbf{S}^{-1}\mathbf{Y}\mathbf{S} - \mathbf{S}^{-1}\mathbf{S}', \qquad \mathbf{P}_S = \mathbf{S}^T\mathbf{P}\mathbf{S}, \\ \mathbf{A}_S &= \mathbf{S}^{-1}A\mathbf{S} + (\mathbf{S}^{-1}\mathbf{B}\mathbf{S})(\mathbf{S}^{-1}\mathbf{S}') - \mathbf{S}^{-1}\mathbf{S}'', \\ \mathbf{B}_S &= \mathbf{S}^{-1}\mathbf{B}\mathbf{S} - 2\mathbf{S}^{-1}\mathbf{S}'. \end{aligned} \tag{3.9}$$

The matrix $\mathbf{S}$ is to be chosen in such a way as to make $\mathbf{P}_S$ nondegenerate near the

singularities. (One may even take $\mathbf{S} = \mathbf{P}^{-1/2}$ and $\mathbf{P}_S = \mathbf{1}$; however, this is not convenient.)

The Riccati equation may be further transformed to make the problem more suitable for computations by renormalizing $\mathbf{Y}_S$ and introducing a new independent variable t:

$$\mathbf{Z} = f(x)\,\mathbf{Y}_S\,, \qquad x = \xi(t). \tag{3.10}$$

The resulting equation is

$$d\mathbf{Z}/dt = g(t)[\mathbf{A}_Z + \mathbf{B}_Z\mathbf{Z} - \mathbf{Z}^2], \tag{3.11}$$

where

$$g(t) = f^{-1}\,d\xi/dt, \qquad \mathbf{A}_Z = f^2\mathbf{A}_S\,, \qquad \mathbf{B}_Z = f\,\mathbf{B}_S + f'. \tag{3.12}$$

(b) *Interval* $0 < x < 1$. In view of Eq. (2.21) the simplest choice of S is

$$\mathbf{S} = \begin{pmatrix} x^{-1} & -x^{-2} & 0 \\ 1 & x^{-1} & 0 \\ 0 & 0 & x^{-2} \end{pmatrix}. \tag{3.13}$$

Now $\det \mathbf{P}_S$ is finite at $x \to 0$, $\mathbf{A}_S \sim x^{-2}$, $\mathbf{B}_S \sim x^{-1}$. Evidently, $\mathbf{Y}_S \sim x^{-1}$ corresponding to a power behavior of the test functions near zero. So, in Eqs. (3.10)–(3.12) we used

$$f(x) = x, \qquad x = t, \qquad g(t) = t^{-1}, \tag{3.14}$$

and $\mathbf{A}_Z$ and $\mathbf{B}_Z$ are finite.

(c) *Interval* $1 \leqslant x < \infty$. At $x \to \infty$,

$$P_{11} \sim x^{3/2}, \qquad P_{12} = P_{21} \sim \tfrac{1}{3}x^{1/2}, \qquad P_{22} \sim \tfrac{1}{5}x^{-1/2}, \qquad P_{33} \sim (2/15)\,x^{7/2}. \tag{3.15}$$

Matrices $\mathbf{A}$ and $\mathbf{B}$ in Eq. (3.4) are of the indeterminate form ∞/∞. To evaluate it, take the diagonal $\mathbf{S}$ with elements

$$S_{11} = x^{-3/4}, \qquad S_{22} = x^{1/4}, \qquad S_{33} = x^{-7/4}. \tag{3.16}$$

Then $\det P$ is finite at large x, $\mathbf{A}_S \sim x^{-3/2}$, $\mathbf{B}_S \sim x^{-1}$, $\mathbf{Y}_S \sim x^{-3/4}$, corresponding to the essential singularity in the test functions, Eq. (2.16). It is natural now to use

$$f(x) = x^{3/4}, \qquad \xi(t) = t^{-4}, \qquad g(t) = -4t^{-2}, \qquad 0 < t \leqslant 1. \tag{3.17}$$

$\mathbf{A}_Z$ is finite $\mathbf{B}_Z \sim t$, $\mathbf{Z}$ is analytical and may be expanded in powers of t near zero.

3.3. *The Calculation*

The process of calculation was as follows. The parameters ζ and R are present in the matrix $\mathbf{Q}$ only,

$$\mathbf{Q}(x) = \zeta^2\mathbf{Q}^{(1)}(x) + \zeta R\mathbf{Q}^{(2)}(x) + \mathbf{Q}^{(3)}(x). \tag{3.18}$$

First of all, the matrices $\mathbf{P}$, $\mathbf{Q}^{(1)}$, $\mathbf{Q}^{(2)}$, $\mathbf{Q}^{(3)}$, and $\mathbf{R}$ were expanded in x near zero and in x^{-1} at infinity. This is a simple task as they are determined by elementary functions (see Appendix). Then, using Eq. (3.11), expansions of $\mathbf{Z}$ were obtained in powers of x near zero and in powers of $t = x^{-1/4}$ at infinity. The first step in doing this was to solve the equation of the form (3.6). Fortunately, in both the cases it may be reduced to the form with $\mathbf{B}_1 = 0$. Besides, at $x \to \infty$, $\mathbf{A}_1$ is the identity multiplied by $\zeta R/4$. The necessary solutions are

$$\mathbf{Z}_1 = \mathbf{G}^{-1}\mathbf{U}\mathbf{G} \qquad \text{at} \quad x \to 0, \tag{3.19}$$

$$\mathbf{Z}_1 = -\tfrac{1}{2}(\zeta R)^{1/2}\,\mathbf{1} \qquad \text{at} \quad x \to \infty, \tag{3.20}$$

where $\mathbf{U}$ is a diagonal matrix with elements

$$U_{11} = \tfrac{1}{2}[1 + (4 - \zeta^2)^{1/2}], \qquad U_{22,33} = \tfrac{1}{2}[1 + (10 \mp 12^{1/2} - \zeta^2)^{1/2}], \tag{3.21}$$

and $\mathbf{G}$ is a matrix diagonalyzing $\mathbf{A}_1$ and independent on ζ and R. The eigenvalues (3.21) are related to the leading powers in expansion of functions φ_k; the first of them is the least and is physically meaningful (cf. Eq. (2.15)), others are specific for the (2, 1) approximation. Note that a positive value was taken for every square root in (3.21) while the minus in Eq. (3.20) guarantees the decreasing at infinity (cf. Eq. (2.16)). Higher coefficients in expansion of $\mathbf{Z}$ (matrices $\mathbf{Z}_2$, $\mathbf{Z}_3$,...) were found with no trouble by solving a chain of linear matrix equations of the general form $\mathbf{CZ} + \mathbf{ZD} = \mathbf{F}$. The necessary number of terms in the expansions is determined by the choice of the starting points x_0 and $x_\infty = t_0^{-4}$. The minimal numbers are 2 at $x \to 0$ and 3 at $t \to 0$ due to the factors of x^{-1} and t^{-2} in Eq. (3.11).

Starting from $x_0 = 0.1$ and $t_0 = 0.1$ with the initial values of $\mathbf{Z}$ given by the expansions (six terms were used) the Riccati equation (3.11) was solved by means of the Runge–Kutta method and the matrices $\mathbf{Z}^{(0)}(1)$ and $\mathbf{Z}^{(\infty)}(1)$ were obtained. Reversing the $\mathbf{S}$ transformation of Section 3.2, one is able to calculate the function $\Delta(\zeta, R)$ in Eq. (3.7). The function $\Delta(\zeta, R)$ is rather sensitive to R near its zero (the derivative $\sim$10–20) providing with a good accuracy in finding R_{cr}. As there is no sharp behavior in the coefficient functions the step in the Runge–Kutta procedure may be as much as 0.01 while the accuracy in $\Delta(\zeta, R)$ is $\sim$0.0001. So, the program does not take more than a few minutes to calculate R_{cr} for a fixed ζ with accuracy 10^{-4}.

IV. Results

The calculations were fulfilled for nuclei with $Z = 90$–100 for $(m, n) = (1, 0)$, $(2, 0)$, $(1, 1)$, $(2, 1)$ as defined in Eq. (2.11). The results are presented in Fig. 1. Evidently, the account for both components of the spinor wavefunction is essential while addition of extra powers of y increases R_{cr} by small corrections. In principle, it is not difficult to calculate a next approximation, e.g., (2, 2); however, it would

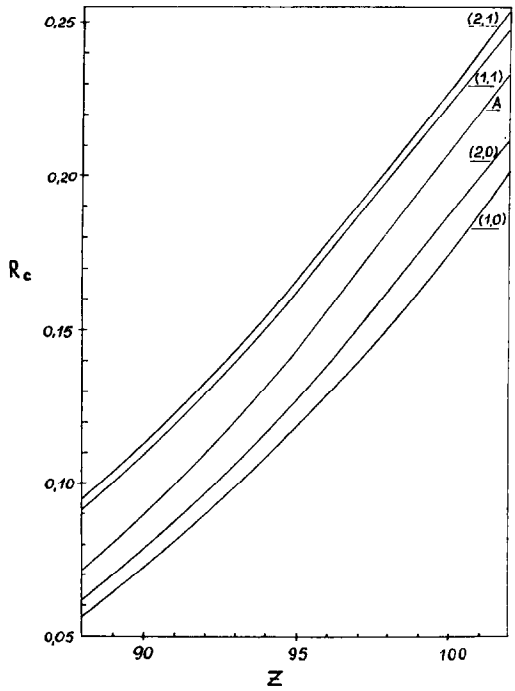

FIG. 1. Various (m, n) approximations for R_{cr} as functions of the nuclear charge. Curve A is calculated by means of Eq. (4.1) based on the asymptotical approach [14].

TABLE I

Various Approximations for R_{cr} (fermi) in case of two Uranium nuclei

			(1, 0)				
Sphere	Müller *et al.* [11]	Asympt.	*a*	*b*	(2, 0)	(1, 1)	(2, 1)
34.3	36	42.8	34.0	34.7	37.4	50.2	51.3

scarcely change R_{cr} by more than 1%–2%. Note that due to the variational principle the calculated values of R_{cr} are the lower limit for the critical internuclear distance.

To illustrate the situation various approaches to calculation of R_{cr} in case of uranium nuclei ($Z = 92$) are presented in Table I. Besides our (m, n) approximations, the following numbers are given: critical diameter of a spherical shell with total charge $2Z$, results of the calculation [11] fulfilled by means of the Ritz method, R_{cr} calculated using the asymptotic formula (4.1) derived in Ref. [14]. The approach with one test function (1, 0) is given for two choices of the variables: (a) Eq. (2.13), (b) Eq. (2.14). This case is considered in some detail in a previous work [16]. Note that the result of the work by Muller, Rafelski, and Greiner [11] is essentially lower than our (2, 1) approximation. The authors considered an expansion of the Ψ function over some set of basis functions used in the nonrelativistic two-center problem (100 basis functions were retained). However, the basis functions have no correct singularity (2.15) near the nuclei and this is an evident reason for a slow convergence of such an approach. By virtue of the variational principle the exact values of R_{cr} are higher than the curve (2, 1) in Fig. 1.

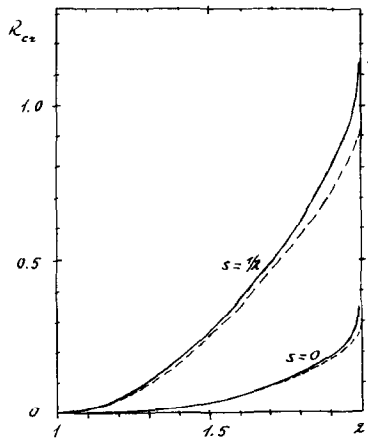

FIG. 2. Critical distance in the two-center problem for pointlike nuclei; R_{cr} in units h/mc, $\zeta = 2Z\alpha$. The dashed curves are calculated by means of Eq. (4.1). The results for a spinless particle are also shown. In this case the abscissa is $Z\alpha$.

The general character of dependence of R_{cr} on ζ is presented in Fig. 2 on the basis of the (2, 1) approximation. We have also shown the curve for the model problem of a scalar particle. This problem, formulated in terms of the Klein–Gordon equation, is quite like the electron problem from the mathematical point of view.

The functional to be variated may be obtained from Eq. (2.9) by putting $\chi_2 \equiv 0$ and omitting the term $\frac{3}{2}\mathbf{F}^2$ in U_{11}. The approximation with one test function is considered in Ref. [16]. Now we have calculated the (2, 0) approximation. The results for R_{cr} differ by no more than 10^{-3}. The dashed curves are calculated using the formulas deduced from analysis of asymptotics [12, 14] at $R_{cr} \ll 1$,

$$R_{cr} = \zeta^{-1} \exp\{-g^{-1}[\operatorname{arc\,ctg}(h/g) - \arg \Gamma(1 + 2ig)]\}, \tag{4.1}$$

where

$$g = (\zeta^2 - 1)^{1/2}, \qquad g_1 = (4 - \zeta^2)^{1/2}, \qquad h = (\zeta + 1)(\zeta - g_1)/(\zeta + g_1)$$

for $s = \frac{1}{2}$ (electron),

$$g = (\zeta^2 - \tfrac{1}{4})^{1/2}, \qquad h = \tfrac{1}{2} - (1 - \zeta^2)^{1/2}$$

for $s = 0$. This formula was derived at $g \ll 1$; however, its deviation from the exact value is no more than 10%–20% up to $\zeta = 1.8$.

In the calculations we assumed that the nuclei are pointlike. This is correct in case $Z < 137$ and there is no "collapse" in the Coulomb field of one nucleus. The account of the finite nuclear radius r_N diminishes R_{cr} by a correction $\sim r_N^2/R_{cr}$ (detailed consideration is given elsewhere). For the nuclei with $Z = 90$–100 this correction is $\sim$0.5 fm.

The obtained values of R_{cr} are rather large; for uranium R_{cr} is more than $7r_N$. The cross sections are several dozens of millibarns, while no background is highly dangerous (discussion in [4]). Note that, as shown in [3], it is not necessary to collide fully ionized beams; it is possible to use a heavy ion beam and a conventional heavy target. With all this in view one may hope that the experiment will soon be set up.

APPENDIX: Coefficient Matrices

Every matrix element in Eq. (2.17) may be expressed via the basic functions of x and y:

$$\begin{aligned}
p(x, y) &= 4R^{-2}(\rho^2 + z^2) = x(2y + 1) - 1, \\
r(x, y) &= 4R^{-2}\rho^2 = -x^2y(y + 1) + x(2y + 1) - 1, \\
\Delta(x, y) &= (4\rho z/R^2)^2 = x^2y(y + 1)\, r(x, y), \\
q(x, y) &= \tfrac{1}{8}R^2[-V - \tfrac{1}{2}V^2 + \tfrac{3}{8}(\nabla V/V)^2] \\
&= \tfrac{1}{4}\{\zeta R[(1 + y)/x]^{1/2} - \zeta^2(1 + y)/x \\
&\quad + \tfrac{3}{4}x^{-2}[x(1 + y)(4y + 1) - 1]/(1 + y)\}.
\end{aligned}$$

TABLE II

Name	Definition		Expansion	
	$0 < x < 1$	$1 \leqslant x$	$x \ll 1$	$x \gg 1$
$u_n(x)$	$x^{-n-1}[(1+x)^{1/2} - (1-x)^{n+(1/2)}]$	$x^{-n-1}(1+x)^{1/2}$	$x^{-n}[(n+1) - n^2x/2 + \cdots]$	$x^{-n-1}(1 + x^{-1}/2 - x^{-2}/8 + \cdots)$
$v_n(x)$	$(2n+1)^{-1}x^{-n}[1 - (1-x)^{n+(1/2)}]$	$(2n+1)^{-1}x^{-n}$	$\frac{1}{2}x^{1-n}[1 - (2n-1)x/4 + \cdots]$	$(2n+1)^{-1}x^{-n}$
$f_0(x)$	$\ln \dfrac{1 + (1+x)^{1/2}}{1 + (1-x)^{1/2}}$	$\ln [x^{-1/2} + (1 + x^{-1})^{-1/2}]$	$\frac{1}{2}x(1 + 5x^2/24 + \cdots)$	$x^{-1/2}(1 - x^{-1}/6 + 3x^{-2}/40 + \cdots)$
$g_0(x)$	$(1+x)^{-1/2} - (1-x)^{1/2}$	$(1+x)^{-1/2}$	$\frac{1}{2}x^2(1 - x/2 + 5x/8 + \cdots)$	$x^{-1/2}(1 - x^{-1}/2 + 3x^{-2}/8 + \cdots)$
$f_n(x)$	$(2n)^{-1}[u_{n-1} - (2n-1)f_{n-1}]$		$\frac{1}{2}x^{1-n}(1 - nx/2 + \cdots)$	$x^{-1/2-n}\left[\dfrac{1}{(2n+1)} - \dfrac{x^{-1}}{2(2n+3)} + \cdots\right]$
$g_n(x)$	$f_{n-1} - g_{n-1}$		$\frac{1}{2}x^{2-n}(1 - (n+1)x/2 + \cdots)$	$x^{-1/2-n}\left[\dfrac{1}{(2n+1)} - \dfrac{3x^{-1}}{2(2n+3)} + \cdots\right]$
$p_n(x)$	$x(2x f_{n+1} + (x-1)f_n)$		$\frac{1}{2}x^{2-n}(1 - nx/2 + \cdots)$	$\dfrac{x^{3/2-n}}{2n+1}\left[1 + \dfrac{2n-3}{2(2n+3)}x^{-1} + \cdots\right]$
$r_n(x)$	$x^3(f_{n+2} + f_{n+1}) - p_n$		$-x^{4-n}(1/12 - nx/24 + \cdots)$	$-x^{3/2-n}\,2(2n+1)^{-1}(2n+3)^{-1} + \cdots$
$q_n(x)$	$\frac{1}{4}[\xi R v_n - \zeta^2(f_n + f_{n+1}) + \frac{3}{4}(4f_{n+1} + f_n - x^{-1}g_n)]$			

Omitting the irrelevant constant factor one may write

$$p_{ij}(x,y) = \begin{cases} p(x,y)\, y^{i+j-2} & \text{at } i,j \leqslant m, \\ p(x,y)\, \Delta(x,y)\, y^{i+j-2m-2} & \text{at } i,j > m, \\ 0 & \text{at } i \leqslant m, j > m \text{ or } i > m, j \leqslant m. \end{cases}$$

This is the contribution from the gradient terms. Other elements are presented for $m = 2, n = 1$:

$$q_{11} = q(x,y); \qquad q_{12} = q_{21} = yq(x,y);$$
$$q_{22} = y^2 q(x,y) + x^{-2} y(1+y);$$
$$q_{13} = q_{31} = -(8x)^{-1}(4y+1)\, r(x,y);$$
$$q_{23} = q_{32} = -3(8x)^{-1}\, y(1+2y)\, r(x,y);$$
$$q_{33} = \Delta(x,y)[q(x,y) - (4x)^{-1}(1+4y)] + \tfrac{1}{4}[r(x,y) + 2x^2 y(1+y)];$$
$$r_{11} = 0; \qquad r_{21} = 0; \qquad r_{12} = -y(1+y); \qquad r_{22} = yr_{12};$$
$$r_{13} = -r_{31} = -\tfrac{1}{4} yr(x,y);$$
$$r_{23} = -r_{32} = yr_{13};$$
$$r_{33} = x^{-1}\Delta(x,y)\, p(x,y).$$

Integration over y is fulfilled in terms of elementary functions presented in Table II along with the asymptotics. They arise from the pattern integrals

$$f_n, g_n = \tfrac{1}{2} \int_{y_1(x)}^{y_2(x)} y^{n-(1/2)}(1+y)^{-k}\, dy,$$

where $k = \frac{1}{2}$ and $\frac{3}{2}$ for f_n and g_n. For any (m, n) approximation the matrix elements of p, q, r are polynomials in y (except the potential terms $\sim(1+y)^{1/2}$ and $(1+y)^{-1}$ in function $q(x,y)$) and nothing new occurs.

The result for the matrix elements in Eqs. (2.12) and (3.1) is as follows.

$$P_{11} = p_0; \qquad P_{12} = P_{21} = p_1;$$
$$P_{22} = p_2; \qquad P_{13} = P_{31} = P_{23} = P_{32} = 0;$$
$$P_{33} = -x^2[2xr_3 + (3x-1)\, r_2 + (x-1)\, r_1];$$
$$Q_{11} = q_0; \qquad Q_{12} = Q_{21} = q_1; \qquad Q_{22} = q_2 + x^{-1}(f_2 + f_1);$$
$$Q_{13} = Q_{31} = (8x)^{-1}(4r_1 + r_0); \qquad Q_{23} = Q_{32} = (8x)^{-1}\, 3(2r_2 + r_1);$$
$$Q_{33} = -x^2[x^2 q_4 + 2x(x-1)\, q_3 + (x^2 - 3x + 1)\, q_2 - (x-1)\, q_1]$$
$$+ \tfrac{1}{4}[x(4r_3 + 5r_2 + r_1) + r_0 + 2p_0];$$
$$R_{11} = R_{21} = 0; \qquad R_{12} = -x(f_2 + f_1); \qquad R_{22} = -x(f_3 + f_2);$$
$$R_{13} = -R_{31} = \tfrac{1}{4} r_1; \qquad R_{23} = -R_{32} = \tfrac{1}{4} r_2; \qquad R_{33} = x^{-1} P_{33}.$$

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