Critical distance in collision of heavy ions

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A variational calculation of the critical existence R_{cr} between colliding nuclei is carried out. Values of R_{cr} are calculated in the region $90 \leq Z \leq 100$ with allowance for the finite size of the nucleus. It is found that R_{cr} is substantially greater than the nuclear radius r_N (for example, $R_{cr} \approx 50$ *F* for uranium nuclei). The results permit refinement of the prediction of the cross section for spontaneous creation of positrons in Coulomb collisions of heavy nuclei.

1. FORMULATION OF PROBLEM AND DISCUSSION OF RESULTS

In connection with discussion of experiments on spontaneous creation of positrons in collision of heavy nuclei,[1-9] the need arose to solve the two-center problem for the Dirac equation.[10-12] Since the variables in the Dirac equation with a potential $V(\mathbf{r}) = -\alpha(Z_1/r_1 + Z_2/r_2)$ are not separated in any orthogonal coordinate system (in contrast to the nonrelativistic Schrödinger equation, which permits separation in elliptical coordinates ξ, η), it is impossible to obtain a solution in analytic form. At the same time the results of the calculation (and particularly the critical distance R_{cr}) are important for formulation of the experiment, since the positron production cross section, the positron energy spectrum, and the very possibility of performing the experiment with heavy nuclei known at the present time, depend greatly on the numerical value of R_{cr} (see refs. 5 and 6 for more detail).

We recall that R_{cr} is the value of the internuclear distance R at which the energy of the ground-state term of the quasimolecule (Z_1, Z_2, e) crosses the boundary of the lower continuum. Since the nuclear velocity $v_N \ll c$, the electronic terms can be calculated in the adiabatic approximation, i.e., for stationary nuclei. In this article we report results of a numerical solution of the relativistic two-center problem. Calculation of R_{cr} was carried out by a variational method.[10,13] Here, as has already been noted,[10] to obtain satisfactory accuracy it is necessary that the trial functions correctly transmit the nature of the singularity of the exact solution near the nuclei and at infinity.

The form of the singularities of the exact solution is found in Sec. 2. In Sec. 3 we consider the two-center problem for spin s = 0 (the Klein-Gordon equation). In this case, which is considerably simpler in the calculational aspect than the case s = 1/2, it is convenient to investigate the questions of the selection of the class of trial functions and the rapidity of convergence of the variational method. In Sec. 4 we present the results of calculation of R_{cr} for s = 1/2 (an electron in the field of two heavy nuclei); here the nuclei are assumed to be pointlike. In Sec. 5 it is shown that for $Z < 137$ allowance for the finite size of the nucleus can be carried out by perturbation theory, and the corresponding change in R_{cr} is found. The final values of the critical distance are given in Table I. The calculation of R_{cr} in a certain sense completes the theoretical investigation[1-6,12-15] of phenomena occurring in a supercritical Coulomb field and permits prediction of the absolute cross section for spontaneous creation of positrons.

TABLE I

Nucleus	Z	R_{cr}, F	ΔR_{cr}, F	E_t, MeV	σ_1, mb
Th	90	43.2	0.43	540	37
U	92	51.0	0.38	480	66
Pu	94	59.5	0.32	430	110
Cm	96	68.3	0.29	390	178
Cf	98	77.7	0.26	360	278
Fm	100	87.8	0.23	330	420

A somewhat unexpected result (not obvious before numerical calculations were carried out) is the comparatively large value of the critical distance for uranium and nearby nuclei. In this region R_{cr} is 5–10 times the nuclear radius r_N, in spite of the fact that the supercriticality parameter $\delta = (2Z - Z_c)/Z_c$ is still small ($0.06 < \delta < 0.17$ for $90 \leq Z \leq 100$). Naturally, this facilitates the performance of the experiment.

The spontaneous creation of positrons in collisions of heavy ions occurs for an energy E of the incident nucleus (in the laboratory system) greater than a threshold energy E_t:

$$E > E_t = 2(Ze)^2/R_{cr}. \tag{1.1}$$

Values of E_t may be found in Table I; we note that $E_t/A \approx 1-2$ MeV/nucleon. In the approximation of low supercriticality ($\delta \ll 1$) the total cross section for spontaneous positron production is factorized:[5]

$$\sigma(E, Z) = \sigma_1 F(E/E_t). \tag{1.2}$$

The factor σ_1 depends only on the nuclear charge Z and increases rapidly in the interval Z = 90–100 (see Table I). With increasing Z the threshold energy E_t decreases. For these reasons it is desirable to perform the experiment with the heaviest possible nuclei. In Eq. (1.2) we have designated by F the universal function of the ratio $\eta = E/E_t$ calculated by us previously.[6] At threshold ($\eta \to 1$) the function $F(\eta)$ is exponentially small—here the Coulomb barrier for slow positrons appears. Therefore in the threshold region it is difficult to observe spontaneous creation of e^+. However, with increase of η this smallness rapidly disappears, and for $\eta > 3$ the function $F(\eta)$ varies from 0.5 to 1. The cross section for spontaneous production of e^+ in this region amounts to tens of millibarns—see Fig. 1.

To observe this effect it is not necessary to have collision of beams of completely stripped (bare) nuclei. As noted earlier,[4,5] an experiment can be set up with a beam of bare nuclei Z_1 incident on an ordinary heavy target Z_2 if $Z_1 \geq Z_2$. Obviously it is necessary to detect not only the positrons but also the nuclei, fixing the scattering angle θ. Here a sharp peak will be observed

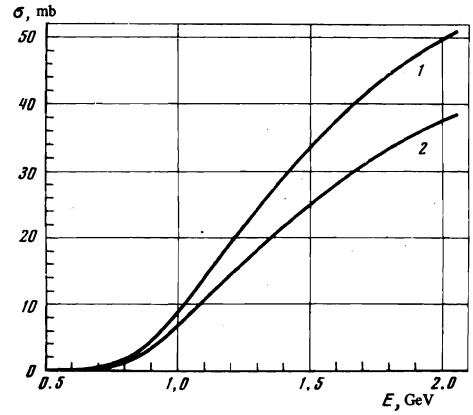

FIG. 1. Cross section for spontaneous production of positrons in slow collisions: 1—two bare uranium nuclei, 2—bare nucleus with a neutral atom ($Z_1 = Z_2 = 92$).

in the energy spectrum of the created positrons near the upper end of the spectrum.[6,9]

Since new heavy-ion accelerators[16,17] will be coming into operation in the coming years, we can expect that this experiment will be carried out in the near future. Observation and study of spontaneous creation of positrons would mean a complete verification of quantum electrodynamics in strong external fields.[1,18]

Here and subsequently $\hbar = c = m = 1$, ϵ is the energy of the level in units of mc^2, R is the distance between nuclei, r_N is the nuclear radius, $\alpha = e^2/\hbar c = 1/137$, $\xi = 2Z\alpha$. To simplify the calculations we will limit ourselves to the case of identical nuclei: $Z_1 = Z_2 = Z$.

2. THE ASYMPTOTE OF $\Psi(r)$ AT SMALL AND LARGE DISTANCES

We will determine the behavior of the wave function near the nuclei and for $r \to \infty$ ($\mathbf{r} = (\mathbf{r}_1 + \mathbf{r}_2)/2$, r_i is the distance from the electron to the i-th nucleus). We will begin with the case $r \gg R$.

In this region the potential of the two-center problem approaches spherical symmetry:

$$V(\mathbf{r}) = -\frac{\xi}{2}\left(\frac{1}{r_1}+\frac{1}{r_2}\right) = -\frac{\xi}{r}\left[1+\left(\frac{R}{2r}\right)^2 P_2(\cos\theta)+\dots\right].$$

For a scalar particle at $\epsilon = -1$

$$(\Delta - 2U_0)\psi = 0,$$
$$U_0 = -V - \frac{1}{2}V^2 = \frac{\xi}{r} - \frac{\xi^2}{2r^2} + \frac{\xi R^2}{4r^3}P_2(\cos\theta) + O(r^{-4}). \tag{2.1}$$

Corresponding to this we will set $r\psi = \chi_0 + \chi_2 P_2(\cos\theta) + \dots$ Substituting this series into (2.1), with accuracy to a common factor (determined by normalization) we find

$$\chi_0(r) = \exp(-\sqrt{8\xi}r)\, r^{1/4}\{1 + c_1 r^{-1/2} + \dots\},$$
$$\chi_2(r)/\chi_0(r) = (R/2r)^2\{1 + c_2 r^{-1/2} + \dots\}, \tag{2.2}$$

where c_1 and c_2 are certain constants.

The case spin 1/2 is somewhat more complicated. The squared Dirac equation at the boundary of the lower continuum reduces to the form (2.1), where now[2,14] U_0 is replaced by $U_{1/2}$:

$$U_{1/2} = -V - \frac{1}{2}V^2 - \frac{1}{4V}\Delta V + \frac{3}{8V^2}(\nabla V)^2 - \frac{1}{2V}[\nabla V \times \mathbf{p}]\sigma. \tag{2.3}$$

The first two terms coincide with the effective potential for a scalar particle, and the third term vanishes for the two-center problem.[1)] The term proportional to $(\nabla V/V)^2$ describes an additional repulsion which increases the critical charge for $s = 1/2$ in comparison with $s = 0$ for the same value of R. Finally, the last term corresponds to the spin-orbit interaction; its sign is not determined. In a central field $V = V(r)$ this term vanishes for the ground state:

$$-\frac{1}{2V}[\nabla V \times \mathbf{p}]\sigma = -\frac{V'}{2rV}(\mathbf{l}\sigma) = (\varkappa + 1)\frac{V'}{2rV},$$

since $\kappa = -1$. Therefore in the two-center problem this term is small both for $r \gg R$ and near each of the nuclei (i.e., in the same regions where the potential approaches spherical symmetry).

Discarding terms smaller than r^{-3} as $r \to \infty$, we have

$$\Delta\psi - \left\{\frac{2\xi}{r} - \frac{\xi^2 - 3/4}{r^2} + \frac{\xi R^2}{2r^3}P_2(\cos\theta) + \frac{i}{r^2}\left(\sigma_\varphi\frac{\partial}{\partial\theta} - \frac{\sigma_\theta}{\sin\theta}\frac{\partial}{\partial\varphi}\right)\right\}\psi = 0, \tag{2.4}$$

where

$$\sigma_\theta = (\sigma_x\cos\varphi + \sigma_y\sin\varphi)\cos\theta - \sigma_z\sin\theta,\quad \sigma_\varphi = -\sigma_x\sin\varphi + \sigma_y\cos\varphi.$$

In matrix form

$$\sigma_\theta = \begin{pmatrix} -\sin\theta & \cos\theta e^{-i\varphi} \\ \cos\theta e^{i\varphi} & \sin\theta \end{pmatrix},\quad \sigma_\varphi = \begin{pmatrix} 0 & -ie^{-i\varphi} \\ ie^{i\varphi} & 0 \end{pmatrix}.$$

We will seek a solution of Eq. (2.4) in the form

$$\psi(\mathbf{r}) = \frac{1}{r}\begin{pmatrix} \psi_0(r) + \psi_1(r)P_2(\cos\theta) + \dots \\ \psi_2(r)\sin 2\theta\, e^{i\varphi} + \dots \end{pmatrix}. \tag{2.5}$$

Substituting (2.5) into (2.4), we arrive at a system of equations,

$$\psi_0'' - \left(\frac{2\xi}{r} + \frac{3/4 - \xi^2}{r^2}\right)\psi_0 = 0,$$
$$\psi_1'' - \left(\frac{2\xi}{r} + \frac{27/4 - \xi^2}{r^2}\right)\psi_1 = \frac{4}{r^2}\psi_2 - \frac{\xi R^2}{2r^3}\psi_0,$$
$$\psi_2'' - \left(\frac{2\xi}{r} + \frac{31/4 - \xi^2}{r^2}\right)\psi_2 = \frac{3}{2r^2}\psi_1,$$

whose solution for a bound level ($\psi \to 0$ as $r \to \infty$) asymptotically has the form

$$\psi_0(r) = Cr^{1/4}\exp(-\sqrt{8\xi}r),$$
$$\psi_1/\psi_0 = -1/3(\xi R)^{1/2}(R/2r)^{1/2},\quad \psi_2/\psi_0 = -1/8(R/2r)^2. \tag{2.6}$$

In the region near the nuclei the wave equation can conveniently be analyzed in elliptical coordinates

$$\xi = (r_1 + r_2)/R,\quad \eta = (r_1 - r_2)/R, \tag{2.7}$$

which are usually used in the nonrelativistic two-center problem ($1 \le \xi < \infty$, $-1 \le \eta \le 1$; the nuclei correspond to the point $\xi = 1$, $\eta = \pm 1$). Leaving the most singular terms in the Klein-Gordon and Dirac equations, we can show[10] that the solutions have singularities of the form

$$\psi(\mathbf{r}) \sim (\xi^2 - \eta^2)^{-\sigma/2},\quad \sigma = 2s + 1 - [(2s+1)^2 - \xi^2]^{1/2}, \tag{2.8}$$

where $s = 0, 1/2$ is the spin of a particle moving in the field of two centers. This singularity $\psi \sim (r_1 r_2)^{-\sigma/2}$ disappears in the transition to the nonrelativistic case: $\sigma \to 0$ for $Z \ll 137$.

We note further that the solution of the squared Dirac equation for the Σ term is of the form

$$\psi(\mathbf{r}) = \begin{pmatrix} \chi_1(\xi,\eta) \\ \chi_2(\xi,\eta)e^{i\varphi} \end{pmatrix}. \tag{2.9}$$

The functions χ_1 and χ_2 correspond to the projections of the orbital angular momentum $\Lambda = 0, 1$ on the axis of the quasimolecule (the z axis), and φ is the angle of rotation around this axis. Here $\chi_2 \sim \rho$ as $\rho \to 0$, where $\rho = (1/2)R[(\xi^2 - 1)(1 - \eta^2)]^{1/2}$ is the distance to the

z axis (this behavior of χ_2 is a particular case of the relaxation $\chi \sim \rho^{|\Lambda|}e^{i\Lambda\varphi}$ for states with angular-momentum projection Λ). In the case $Z_1 = Z_2$ the wave function of the ground-state term does not change for the substitution $r_1 \leftrightarrow r_2$ ($\xi \to \xi$, $\eta \to -\eta$, $\varphi \to \varphi + \pi$), and hence in Eq. (2.9)

$$\chi_k(\xi, -\eta) = (-1)^{k-1}\chi_k(\xi, \eta); \; k=1, 2. \tag{2.10}$$

3. CRITICAL DISTANCE R_{cr} FOR A SCALAR PARTICLE. CHOICE OF THE CLASS OF TRIAL FUNCTIONS

Solution of the Klein-Gordon equation for an energy $\epsilon = -1$ is equivalent to finding the minimum of the functional

$$J[\psi] = \int d^3r\left(\tfrac{1}{2}|\nabla\psi|^2 + \psi^+ U_0\psi\right), \tag{3.1}$$

where $U_0 = -V - (1/2)V^2$ is the effective potential and ψ is the trial function. The equation for ψ is obtained by variation of $J[\psi]$ within the limits of the selected class of trial functions. If no limitations are imposed on ψ, then for exact determination of R_{cr} it is necessary to solve the equation in partial derivatives in the ξ, η plane (see Eq. (19) in ref. 10), which is an extremely difficult problem. Below we use an approximate method, the idea of which is as follows. Instead of ξ and η we will introduce new variables

$$x = x(\xi, \eta), \quad y = y(\xi, \eta). \tag{3.2}$$

In the case of separation of the variables, the choice of x and y is obvious—the solution is factorized: $\psi(x, y) = \psi_1(x)\psi_2(y)$. For example, for a potential with spherical symmetry we have $x = r$, $y = \theta$. In the relativistic two-center problem, where there is no separation of variables, we will choose x, y so that $\psi(\mathbf{r})$ has a singularity only in x (these coordinates can be called asymptotically separated). Substituting in Eq. (3.1)

$$\psi(\xi, \eta) = \sum_{i=1}^{N} \varphi_i(x) y^{i-1}, \tag{3.3}$$

where φ_i are arbitrary functions of x, after integration over y we have

$$J_N[\psi] = \sum_{i,j=1}^{N} \int dx\left(P_{ij}\varphi_i'\varphi_j' + Q_{ij}\varphi_i\varphi_j + 2R_{ij}\varphi_i'\varphi_j\right). \tag{3.4}$$

Minimization of J_N over the trial functions $\varphi_i(x)$ leads to a system of N equations:

$$\frac{d}{dx}\left(P\frac{d\varphi}{dx} + R\varphi\right) - \tilde{R}\frac{d\varphi}{dx} - Q\varphi = 0 \tag{3.5}$$

(in matrix designations; here $\tilde{R}$ is a matrix transposed to R). Here P(x) and Q(x) are symmetric matrices: $\tilde{P} = P$, $\tilde{Q} = Q$. The solution of the equation in partial derivatives is replaced by a boundary value problem for the system of N ordinary differential equations. The convergence of the method for a correct choice of the variable x turns out to be extraordinarily rapid, as a result of the following:

1) The functional $J_N[\psi]$ is varied over the entire class of functions $\varphi_i(x)$, i.e., the trial function $\psi(\xi, \eta)$ is chosen with an infinite number of variation parameters;

2) The behavior of $\varphi_i(x)$ near the singular points (the ends of the interval of integration over x) is not imposed externally, but is determined by Eq. (3.5) itself.

Let us turn to the choice of the important variable x. With allowance for the nature of the singularities of $\psi(\xi, \eta)$ determined in the previous section, we tried two asymptotically separable coordinate systems. System (a) is

$$x = \frac{\xi^2 - \eta^2}{2\xi} = \frac{2r_1r_2}{R(r_1+r_2)}, \quad y = \frac{\eta^2}{\xi^2}. \tag{3.6}$$

In this system, curves $x(\xi, \eta) = \text{const}$ are essentially equipotentials:

$$V = -\frac{\zeta}{2}\left(\frac{1}{r_1} + \frac{1}{r_2}\right) = -\frac{\zeta}{Rx}.$$

System (b) is

$$x = \xi^2 - \eta^2 = \frac{4r_1r_2}{R^2}, \quad y = \frac{\eta^2}{\xi^2 - \eta^2}. \tag{3.7}$$

In both cases x varies over the interval $(0, \infty)$, at the ends of which the system (3.5) has singularities. Near the nuclei we have $x \sim r_1r_2$, and at infinity x depends only on r. As far as y is concerned, $y \approx r^{-2}\cos^2\theta$ as $r \to \infty$, and therefore inclusion of N terms of the series (3.3) corresponds to expansion of $\psi(\mathbf{r})$ in Legendre polynomials $P_{2n}(\cos\theta)$ up to $n = N - 1$. The results of the calculation are given in Table II.

TABLE II. Values of R_{cr} (in units of $\hbar$/mc) for scalar particle

$\zeta = 2Z\alpha$	$x = \xi$, $N = 1$	$x = (\xi^2-\eta^2)/2\xi$, $N = 1$	$x = \xi^2 - \eta^2$	
			$N = 1$	$N = 2$
0.70	0.012	0.0132	0.0141	0.0141
0.75	0.026	0.0289	0.0296	0.0297
0.80	0.048	0.0521	0.0534	0.0535
0.85	0.076	0.0836	0.0856	0.0858
0.90	0.109	0.1252	0.1281	0.1282
0.95	0.147	0.1815	0.1853	0.1853

Values of R_{cr} were calculated first with one trial function (N = 1), but with various choices of the variable x. The larger the calculated value of R_{cr} for a given ζ, the better the selection of x. Variants a) and b) lead to extremely similar results. For comparison we have also given the values of R_{cr} obtained [19] for $x = \xi$. This choice of x does not permit determination of the nature of the singularity of (2.8) and has significantly poorer accuracy. Hence it is evident that the condition of asymptotic separability of the variables x, y is important.

Retaining the best variant $x = \xi^2 - \eta^2$, we investigated the convergence of the expansion (3.3). The transition from N = 1 to N = 2 corresponds to inclusion of the quadrupole correction $\chi_2(r)P_2(\cos\theta)$. Here the value of R_{cr} increased by no more than 0.2%. This indicates the extraordinarily rapid convergence of this method.

The values of R_{cr} calculated here give a lower limit for the critical distance between the nuclei. Suppose the expansion (3.3) with N terms (a polynomial of degree $N - 1$ in y) gives a value $R_{cr}^{(N)}$. Then $R_{cr}(\zeta) = \lim R_{cr}^{(N)}(\zeta)$ as $N \to \infty$, where

$$R_{cr}^{(1)}(\zeta) < R_{cr}^{(2)}(\zeta) < R_{cr}^{(3)}(\zeta) < \ldots. \tag{3.8}$$

Actually, equation (2.1) for the Σ term is equivalent to the problem of appearance of the first bound level in the effective potential U_0. If R is fixed, the coupling constant ζ increases. In view of the variational principle, $\zeta_c^{(N)}(R) > \zeta_c^{\text{exact}}(R)$. If we take into account the fact that the curve $\zeta_c = \zeta_c(R)$ increases monotonically, the inequality (3.8) follows. On increasing the number of terms N in the expansion (3.8), the corresponding values of $R_{cr}^{(N)}$ rise monotonically, approaching a limit $R_{cr}(\zeta)$ from below.

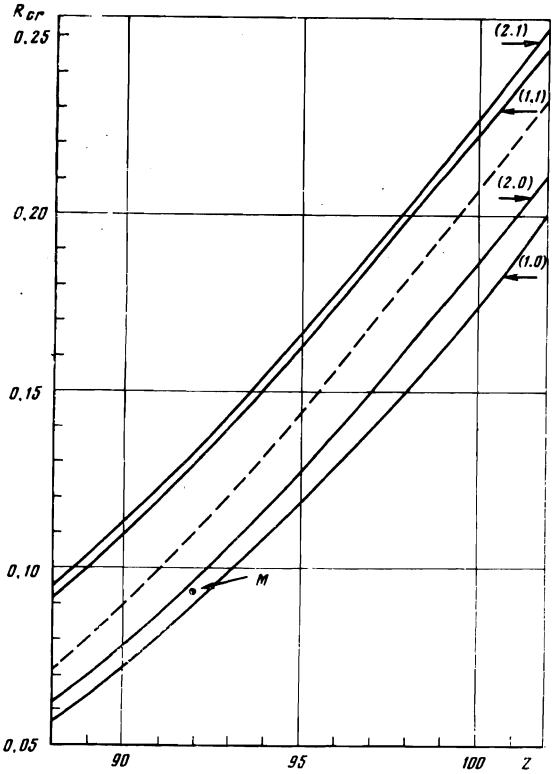

FIG. 2. Critical distance in the two-center problem (R_{cr} in units of $\hbar/mc$ = 386 F). The numbers on the curves indicate the order of the approximation (m, n) in Eq. (4.2). The dashed curve is the asymptotic solution obtained in ref. 14.

4. CRITICAL DISTANCE IN COLLISION OF NUCLEI

For a particle with spin 1/2 the calculations are significantly more complicated. The functional $J[\psi]$ as before has the form (3.1), but the effective potential U_0 must be replaced by $U_{1/2}$, which depends on the spin variables (see Eq. (2.3)). Here the trial function ψ is a two-component spinor having the structure (2.9). Integrating $J[\psi]$ over the angle of rotation around the quasimolecule axis (the z axis) we find

$$J[\psi]=\text{const}\cdot\int_0^\infty \rho d\rho\int_0^\infty dz\left\{\frac{(\partial\chi_1)^2+(\partial\chi_2)^2}{2}+U_{11}\chi_1^2+2U_{12}\chi_1\chi_2+U_{22}\chi_2^2+\chi_1\hat{\Lambda}\chi_2-\chi_2\hat{\Lambda}\chi_1\right\}, \tag{4.1}$$

where ρ and z are cylindrical coordinates,

$$(\partial\chi)^2=(\partial\chi/\partial\rho)^2+(\partial\chi/\partial z)^2,$$
$$U_{11}=-V-{}^1/_2V^2+{}^3/_2\mathbf{F}^2,\quad U_{12}=F_z/\rho,$$
$$U_{22}=U_{11}+\frac{1}{\rho}F_\rho+\frac{1}{2\rho^2},\quad \hat{\Lambda}=F_z\frac{\partial}{\partial\rho}-F_\rho\frac{\partial}{\partial z},$$
$$\mathbf{F}=\frac{1}{2V}\nabla V,\quad F_\rho=\frac{1}{2V}\frac{\partial V}{\partial\rho},\quad F_z=\frac{1}{2V}\frac{\partial V}{\partial z},$$

and V is the potential of the two-center problem. In accordance with the results of Sec. 3, we choose (3.7) as the variables x, y. Taking into account the symmetry properties (2.10), we set

$$\chi_1=\sum_{k=1}^{m}\varphi_k(x)y^{k-1},\quad \chi_2=\frac{4\rho z}{R^2}\sum_{k=1}^{n}\varphi_{m+k}(x)y^{k-1}. \tag{4.2}$$

Substituting χ_1, χ_2 into (4.1) and varying $J[\psi]$ over the trial functions $\varphi_k(x)$, we arrive at a system of N = m + n equations of the type (3.5). This approximation will be called the (m, n) approximation. We note that all coefficients P(x), Q(x), and R(x) of the system (3.5) can be expressed in the form of finite combinations of elementary functions. Omitting the explicit formulas for these coefficients in view of their cumbersome nature, we give here the results of the calculation.

In Fig. 2 we have shown values of R_{cr} calculated in the approximations (m, n) = (1, 0), (2,0), (1, 1), and (2, 1). From comparison of the curves of the (1, 0) and (1, 1) approximations it is clear that taking into account the two components χ_1 and χ_2 of the wave function is extremely important. At the same time the convergence of the expansions (4.2) in powers of y is rather rapid; this is indicated by the transition from the (1, 1) approximation to the (2, 1) approximation. We will limit ourselves to the (2, 1) approximation. However, it is possible by the same method to further improve the values of R_{cr}, by converting to approximations of higher order.[2)] As in Sec. 3, we can show that R_{cr} in this case will increase:

$$R_{cr}^{(m,n)}(\zeta)<R_{cr}^{(m',n')}(\zeta),\qquad \text{if } m'\geqslant m,\ n'\geqslant n, \tag{4.3}$$

approaching from below the exact solution. Indeed, in the transition from the approximation (m, n) to (m′, n′) the class of trial functions (4.2) is expanded, in view of which the result of the variational calculation of R_{cr} is exaggerated. Therefore the values obtained here give a lower limit for the critical distance in the two-center problem. For comparison we have also shown in Fig. 2 the result of calculation of $R_{cr}(\zeta)$ by the method of matching asymptotes[14]—see the dashed curve.

For Z = 92 the critical distance was calculated also by Müller, Rafelski, and Greiner.[11] They utilized an expansion of the wave function in a series in a system of basis functions

$$\psi_{nl}(\xi,\eta)=(\xi^2-1)^{\mu/2}e^{-(\xi-1)/a}L_n^\mu((\xi-1)/a)P_l^\mu(\eta),$$

which leads to rapidly converging results in the nonrelativistic two-center problem. However, these functions do not have the correct singularity (2.8) which is specific for the relativistic Coulomb problem. This may explain the fact that, although in ref. 11 100 terms of the series in ψ_{nl} were retained, the corresponding result (see the point M in Fig. 2) is significantly poorer than the (2, 1) approximation, since the exact values of $R_{cr}(\zeta)$ lie clearly above the (2, 1) curve. Actually the result of ref. 11 is close to our (1, 0) approximation, in which only one trial function is used. This demonstrates the advantages of the method of calculation of R_{cr} used by us, in which the trial functions automatically have the necessary singularities.

5. ALLOWANCE FOR FINITE SIZE OF THE NUCLEI

Up to this time we have discussed the nuclei as point-like. We will now estimate the decrease in R_{cr} on taking into account the nuclear radius r_N. Since $Z < 137$ and $r_N \ll R_{cr}$, the correction for the finite size of the nucleus can be taken into account by perturbation theory (since in the field of one nucleus Z the electron does not experience a falling to the center).

Inside the nucleus ($0 < r < r_N$)

$$V(r)=-(\zeta/r_N)f(r/r_N), \tag{5.1}$$

where the cutoff function f(x) = 1 for cutoff model I and $f(x) = (3-x^2)/2$ for model II. Although only model II is realistic and corresponds to a uniform volume density of electric charge of the nucleus, the calculation of ΔR_{cr} is conveniently begun with model I.

Let $\zeta_c = 2Z_c\alpha$ be the critical charge of the two-center problem with point nuclei. Assuming that the curve $\zeta_c = \zeta_c(R)$ is known, we will show how to find the correction $\Delta\zeta_c$ for finite nuclear size for the condition $r_N \ll R$. Since in perturbation theory ζ_c is a linear functional of the charge-distribution density, in a transition from pointlike nuclei to nuclei charged on the surface (model I) the critical charge increases by an amount

$$\Delta\zeta_c = \int_0^\pi \zeta_c([R^2 + r_N^2 - 2Rr_N\cos\theta]^{1/2})\sin\theta d\theta - 2\zeta_c(R)$$
$$= \frac{1}{Rr_N}\int_{R-r_N}^{R+r_N}[r\zeta_c(r) - R\zeta_c(R)]dr \approx \frac{2r_N^2}{3R}\left[\zeta_c'(R) + \frac{R}{2}\zeta_c''(R)\right]. \quad (5.2)$$

Converting from $\zeta_c(R)$ to the inverse function $R = R_{cr}(\zeta)$, we have

$$\Delta R_{cr}^{\ I} = R'\Delta\zeta_c = \frac{2r_N^2}{3R}\left\{1 - \frac{RR''}{2(R')^2}\right\}. \quad (5.3)$$

Let us turn now from cutoff model I to model II. Near the nuclei the wave function of the two-center problem has a singularity of the type $(r_1r_2)^{-\sigma/2}$—see Eq. (2.8). Hence

$$\Delta\zeta_c = C\int_0^1 dx\left[\frac{1}{x} - f(x)\right]x^{2\gamma}, \quad \gamma = 1 - \frac{\sigma}{2} = [1-(Z\alpha)^2]^{1/2}$$

(the constant C is determined by normalization of the function ψ). Hence it is easy to find the ratio of $\Delta\zeta_c$ and ΔR_{cr} for the two cutoff models:

$$\frac{\Delta R_{cr}^{\ II}}{\Delta R_{cr}^{\ I}} = \frac{\Delta\zeta_c^{\ II}}{\Delta\zeta_c^{\ I}} = \frac{3}{3+2\gamma} \quad (5.4)$$

The values of ΔR_{cr} calculated with these formulas for $r_N = 1.2A^{1/3}$ [F] are listed in Table I. The term containing R″ in Eq. (5.3) makes a contribution amounting to ≈20% of the first term. The values of R_{cr} given in Table I already include the correction for finite nuclear size.

We will make a final remark about the region of applicability of perturbation theory in r_N. For this purpose let us consider a 1s level in a spherical nucleus whose energy for $r_N = 0$ is $\epsilon_0 = [1 - (Z\alpha)^2]^{1/2}$. Inclusion of the cutoff (5.1) increases the energy of this level, which is equivalent to decreasing the point charge by an amount ΔZ:

$$\frac{\Delta Z}{Z} = -\frac{(\zeta r_N)^{2\gamma}}{\Gamma(1+2\gamma)}\left\{1 - 2\gamma\int_0^1 f(x)x^{2\gamma}dx\right\}. \quad (5.5)$$

Perturbation theory assumes $\Delta Z \ll Z$, which leads to the condition $(\zeta r_N)^{2\gamma} \ll 1$. For $r_N = 8$ F and $Z < 100$, we have $(\zeta r_N)^{2\gamma} \lesssim 0.01$, which justifies the use of perturbation theory. On the other hand, near $Z = 137$, where $1 - Z\alpha \sim (-\ln r_N)^{-2}$, the correction ΔZ is comparable with Z and perturbation theory in r_N ceases to be applicable.

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[1)] If $V = q/r$, then $\Delta V = -4\pi q\delta(r)$ and $\Delta V/V \sim r\delta(r) \equiv 0$.

[2)] It is particularly desirable to discuss the (2,2) approximation. We note that the simplest approximation (1,0) was discussed in ref. 15, and the results of a calculation on the basis of the (2,1) approximation have been briefly reported in ref. 12. The numerical solution of the system of Eqs. (3.5) was carried out by conversion to a matrix Y(x) of logarithmic derivatives: $\phi' = Y\phi$. The idea behind this method was suggested in ref. 20.

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