VARIATIONAL CALCULATION OF THE CRITICAL DISTANCE BETWEEN NUCLEI

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A variational calculation is performed of the critical distance R_c between colliding nuclei. In this calculation, the principal term of the quasimolecule (Z, Z, e) drops to the boundary of the lower continuum, and spontaneous production of positrons begins.

In connection with discussions [1 - 4] of spontaneous positron production in collisions of heavy nuclei with charges $Z_1 + Z_2 > Z_c \approx 170$, it has become necessary to solve the two-center problem for the Dirac equation[1)]. The results of this calculation are very important for the planning of experiments, since the production cross section of the positron and their energy spectrum depend strongly on the distance R between nuclei [3, 6]. We recall that the critical distance R_c is defined as that value of R at which the principal term of the quasimolecule (Z_1, Z_2, e) that is produced when the nuclei Z_1 and Z_2 approach each other drops to the limit of the lower continuum $\varepsilon = -1$ (we put henceforth $h = c = m_e = 1$). The quasistatic positron is produced as a result of the dropping of the unfilled level to the lower continuum when the distance between the nuclei decreases to $R < R_c$.

In the physically most important case, that of "small supercriticality" (i.e., under the condition $Z_1 + Z_2 - Z_c \ll Z_c$), all the quantities pertaining to the process of spontaneous positron production are expressed in terms of universal functions of the ratio R/R_c, which have been calculated in explicit form [6]. By the same token, the calculation of R_c completes, in a certain sense, the theory of the phenomena that occur in the supercritical region, and allows us to make the predictions needed for the experiments.

However, the calculation of the critical distance entails considerable mathematical difficulties, since the variables in the Dirac equation with the potential $V(\vec{r}) = -\alpha[(Z_1/r_1) + Z_2/r_2)]$ cannot be separate in any orthogonal coordinate system, and it is impossible here to obtain an analytic solution of the problem. For a numerical calculation of R_c, a variational principle was proposed [7, 8]. We report here the results of numerical calculations performed by the variational method.

As shown in [7, 8], the calculation of R_c is equivalent to a determination of the minimum of the functional

$$J[\psi] = \int d^3r [\,|\nabla\psi|^2 + 2\psi^+ U\psi], \tag{1}$$

where $\psi(\vec{r})$ is a traal function (two-component spinor) and $U(\vec{r})$ is the effective potential in the Dirac equation at the energy $\varepsilon = -1$:

$$U = -\left(V + \frac{1}{2}V^2\right) - \frac{1}{4V}\Delta V + \frac{3}{8V^2}(\nabla V)^2 - \frac{1}{2V}\vec{\sigma}[\nabla V \times \mathbf{p}]. \tag{2}$$

Here $V(\vec{r})$ is the potential that enters directly in the Dirac equation. To simplify the calculations, we put $Z_1 = Z_2 = Z$ (identical nuclei). It follows then from symmetry consideration that the exact solution takes the form

$$\psi(\mathbf{r}) = \begin{pmatrix} \chi_1(\xi, \eta) \\ \chi_2(\xi, \eta)\exp(i\phi) \end{pmatrix}, \tag{3}$$

where ξ, η, ϕ are elliptic coordinates: $\xi = (r_1 + r_2)/R$ and $\eta = (r_1 - r_2)/R$ $(1 \leq \xi < \infty,\ |\eta| \leq 1)$. 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). Then χ_1 and χ_2 are respectively even and odd in η, and in addition χ_2 vanishes on the z axis: $\chi_2 \propto z\rho$, where $z = (1/2)R\xi\eta$, and $\rho = (R/2)\cdot[(\xi^2 - 1)(1 - \eta^2)]^{1/2}$ is the distance to the z axis. To attain good accuracy of the variational calculations of R_c it is necessary that the trial functions account correctly for the character

of the singularity of the exact solution at the singular points corresponding to the Coulomb centers[2], and also at infinity. In this case, the form of the singularities $\psi(\vec{r})$ is known [7] and dictates the choice of the class of trial functions.

Near one of the nuclei we have $\xi^2 - \eta^2 \ll 1$ and $\psi \propto (\xi^2 - \eta^2)^{\sigma}$, where σ depends only on z. Far from the nuclei we have $\xi \gg |\eta|$ and $\psi \propto \exp(-\sqrt{8Z\alpha R}\xi)$. It is therefore more convenient to use the variables $x = \xi^2 - \eta^2$ and

$$x = \xi^2 - \eta^2, \quad y = \eta^2/(\xi^2 - \eta^2) \qquad (0 < x < \infty). \tag{4}$$

We seek the extremum of the functional (1) on the class of trial functions

$$\chi_1 = \phi_1(x) + y\phi_2(x), \quad \chi_2 = R^{-2}\rho z \phi_3(x). \tag{5}$$

Trial functions in this form make it possible to take into account in the vicinity of one of the nuclei ($x \gg 1$) the field of the other nuclei, and to take into account far from the nuclei ($x \gg 1$) the quadrupole correction in the two-center potential.

Substituting (5) in (1) we have

$$J[\psi] = \int_0^{\infty} dx\,(p_{ij}\phi_i'\phi_j' + q_{ij}\phi_i\phi_j + 2r_{ij}\phi_i'\phi_j). \tag{6}$$

Variation of $J[\psi]$ with respect to the arbitrary functions $\phi_i(x)$ leads to the system of equations[3]

$$(p_{ij}\phi_j' + r_{ij}\phi_j)' - r_{ji}\phi_j' - q_{ij}\phi_j = 0. \tag{7}$$

the coefficients p, q, and r can be calculated in explicit form in terms of elementary functions. For example,

$$p_{11}(x) = x[(x-1)f_0 + 2xf_1],$$

where

$$f_0 = \ln\frac{1+\sqrt{1+x}}{1+\sqrt{1-x}}, \quad f_1 = \frac{1}{2x}(\sqrt{1+x} - \sqrt{1-x}) - \frac{1}{2}f_0 \text{ at } 0 < x \leqslant 1,$$

$$f_0 = \ln\frac{1+\sqrt{1+x}}{\sqrt{x}}, \quad f_1 = \frac{1}{2}\sqrt{1+\frac{1}{x}} - \frac{1}{2}f_0 \qquad \text{at } x \geqslant 1.$$

A feature of this method is that the functional $J[\phi]$ is varied on an entire class of functions $\phi_i(x)$, i.e., a trial function is chosen with an infinite number of variational parameters. The dependence of $\psi(\vec{r})$ on the significant variable x, in terms of which a singularity exists, is determined by Eqs. (7) themselves. These circumstances ensure good accuracy of R_c. We note also that by virtue of the variational principle the true values of R_c can only exceed those calculated by us.

In practice, the employed method replaces the solution of the system of two partial differential equations (for χ_1 and χ_2) of the boundary-value problem for the system of ordinary differential equations on the semi-axis $0 < x < \infty$. From the computational point of view, the problem is made somewhat more complicated because the edges of the interval are singular points. A method was found to get around this difficulty (it will be described in a separate article).

The results of the numerical calculations are given in the table. Here $\zeta = 2Z/137$, and $E_t = 2(Ze)^2/R_c$ is the threshold incident-nucleus energy at which spontaneous positron production begins. The total cross section for e^+ production is given by $\sigma(E, Z) = \sigma_0 f(E/E_t)$, where f is a certain universal function calculated in [6]; for example, $f(2) = 1.7\times10^{-4}$. The factor σ_0 determines the dependence of the cross section on Z. We call attention to the rapid growth of σ_0 when Z increases from 90 to 100. The threshold energy E_t is then decreased, by virtue of which it is expedient to perform the experiment with as heavy nuclei as possible. Since R_c is 4 - 5 times larger than the nuclear diameter, the performance of such an experiment seems perfectly realistic.

Nucleus	ζ	R_c, F	E_t, MeV	σ_0, b
Th	1,314	43,5	530	30,8
U	1,343	51,3	475	53,8
Pu	1,372	59,8	425	91,0
Cm	1,401	68,7	385	146,0
Cf	1,431	78,0	355	225,0
Fm	1,460	88,0	330	341,0

[1)] The possibility of production of electron-positron pairs from vacuum in a strong electric field was predicted long ago in quantum electrodynamics, but this effect was not yet observed experimentally. The spontaneous production of e^+ in a Coulomb field with charge $Z > Z_c$ is of interest as a check on the Dirac equation in strong external field and as a check on the properties of physical vacuum [1, 4], and also from the point of view of verifying the linearity of the fundamental equations of quantum electrodynamics.

[2)] Since the charge of each of the nuclei is $Z < 137$, there is no "falling to the center" in a Coulomb field $-Z\alpha/r$, and the nuclei can be regarded as pointlike. The correction for the finite dimensions of the nucleus at $Z = 90$ to 100 increases the energy of the principal term by only $\Delta\varepsilon \sim 1.5\times10^{-3} < 1$ keV (see formula (12) of [9]).

[3)] Repeated indices mean summation. The system (7) has a solution satisfying the boundary conditions (exponential decrease at infinity and smallest singularity as $x \to 0$) exists only for discrete values of R, if $\zeta = 2Z/137$ is fixed. The largest of these three roots determines the $R_c(\zeta)$ dependence for the main term.

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DEEP INELASTIC LEPTON-PROTON SCATTERING AND μ-e UNIVERSALITY

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To verify μ-e universality, a joint analysis was performed of the data on deep inelastic μ-p and e-p scattering. It is shown that these data are compatible if the μ-p-scattering cross sections are renormalized.

We report here the results of a joint analysis of the data on deep inelastic μ-p scattering, obtained in [1], and the data of the SLAC-MIT group [2, 3] on deep inelastic e-p scattering. The main purpose of the analysis was to check on the μ-e universality.

The data of [1] on μ-p scattering were obtained at a muon momentum 12 GeV/c and $q^2 \leq 4$ $(\text{GeV/c})^2$. The e-p scattering cross sections were measured [2, 3] at electron energies up to