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QUANTUM ELECTRODYNAMICS
AND EXOTIC ATOMIC PHENOMENA OF HIGH Z-ELEMENTS *†

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ABSTRACT

We review the physics of the exotic atomic phenomena, especially positron autoionization, which can occur if the charge of the nucleus is increased beyond the critical value $Z \sim 170$. The adiabatic collision of two heavy ions can be used to study experimentally the problem of the Dirac electron in a Coulomb field beyond the critical value where pair production occurs. Various approaches to this phenomenon are discussed, including the possible complications of quantum electrodynamic corrections. A brief review of recent tests of quantum electrodynamics in high Z electronic and muonic atoms is also presented.

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A fascinating problem in atomic physics and quantum electrodynamics is the question of what happens physically to a bound electron when the strength of the Coulomb potential increases beyond $Z\alpha = 1$. This question involves properties of quantum electrodynamics which are presumably beyond the limits of validity of perturbation theory, so it is an area of fundamental interest. Although a complete field theoretic formulation of this strong field problem has not been given, it is easy to understand in a qualitative way what happens physically: As $Z\alpha$ increases beyond a critical value, the discrete bound electron state becomes degenerate in energy with a three-particle continuum state (consisting of two bound electrons plus an outgoing positron wave) and a novel type of pair creation occurs. Remarkably, it may be possible that such "autoionizing" positron production processes of strong field quantum electrodynamics can be studied experimentally.

The earliest discussions of the strong field problem began with the solutions of the Dirac equation for an electron in a Coulomb field. This is of course an idealization since the nucleus is taken as infinitely heavy and point-like and radiation corrections are ignored. The spectrum of the Dirac equation with $V = -Z\alpha/r$ is given by the Dirac-Sommerfield fine structure formula: $\epsilon = \sqrt{1 - (Z\alpha)^2}\, mc^2$ is the binding energy of the ls state. Thus $\epsilon = 0$ appears to be the lower limit of the discrete spectrum as $Z\alpha \to 1$ and ϵ even becomes imaginary for $(Z\alpha) > 1$. Actually, this result is just a mathematical curiosity. As pointed out by Schiff, Snyder and Weinberg[1] in 1940, and also by Pomeranchuk and Smorodinsky,[2] and by Fermi,[3] a boundary condition is required to completely specify the point Coulomb equation. The solutions are well-defined when any nuclear finite size is introduced.

Thus we should consider the "realistic" potentials

$$V = \begin{cases} -\dfrac{Z\alpha}{r}, & r > R \\ -\dfrac{Z\alpha}{r} f\left(\dfrac{r}{R}\right), & r < R \end{cases}$$

where, for example, $f(\rho) = \frac{1}{2}(3-\rho^2)$ for the case of a uniform charge density. The energy eigenvalue is then found by matching the solutions for the Dirac wavefunction at r=R. A qualitatively correct discussion was given in Ref. 2, but accurate extensive calculations were not given until after 1968 by Pieper and Greiner[4] and by Popov.[5] The energy spectrum using the usual nuclear radii is shown in Fig. 1. In Fig. 2, Popov's[5] result for the dependence of $(Z\alpha)_{crit}$ on the nuclear cutoff radius R is shown. It is clear that the "limit point" $\epsilon = 0$ of the point nuclear case is artificial: at sufficiently large $Z\alpha$, ϵ reaches $-mc^2$ for any $R > 0$.

In order to understand what happens physically when Z is increased beyond the critical value $Z_{crit} \sim 170$, where ϵ "dives" below $-mc^2$, we must leave the confines of the single-particle Dirac equation. For the moment we shall ignore the higher order QED effects from electron self-energy corrections and vacuum polarization. (This can always be done mathematically — if we envision taking α small with $Z\alpha$ fixed.) Clearly, the new phenomena involve pair creation since the potential energy in V is sufficient to produce e^+e^- pairs; in fact, if we had a state $|e_-\rangle = a^+_{1s}|0\rangle$ with $\epsilon_{1s} < -mc^2$, then it would be degenerate in energy with the three-particle state $|e_-e_-e_+\rangle = a^+_{1s}a^+_{1s}b^+|0\rangle$ if ϵ_+ (the energy of the positron) $= -\epsilon_{1s} > mc^2$. [The positron thus has a normal energy in the positive continuum.] The true state of the physical problem is thus a combination of the two types of states $|e_-\rangle$ and $|e_-e_-e_+\rangle$. An analogy with Auger or autoionizing states is evident. This state is not discrete, and the single particle energy is effectively complex, corresponding to a decaying state. The proper description of the state requires field theory, and the quantized Fock states of quantum electrodynamics. Although a complete, consistent formulation of quantum electrodynamics for the strong field problem has not yet been given, the essential elements are understood. It is interesting to note that when $Z > Z_{crit}$ a state with two ls bound electrons is lower in energy than the state containing no electrons bound to the field. Thus as emphasized by Fulcher and Klein,[6] the two particle state is the natural choice of a "vacuum" or reference state for excitation.

It would be very exciting if the physical realization of an electron bound to a strong field with Z greater than Z_{crit} could be feasible experimentally. In papers by Müller, Peitz, Rafelski, and Greiner,[7] and by Gershtein and Zeldovitch,[8] the collision of two heavy ions with $Z_1+Z_2 > Z_{crit}$ is considered. The velocity is assumed to be sufficient to overcome the Coulomb barrier, and that, at least adiabatically, a ground state electron sees an effective nuclear potential with $R < R_{crit}$. Let us suppose that only one ground-state electron is present. Then, as the ions collide, the lowest eigenstate becomes mixed with the $|e_- e_- e_+\rangle$ continuum level. As the ions recede, we are left with two electrons in the ls level plus an outgoing positronium state with an angular distribution reflecting the charge density of the colliding nuclei. Note that double pair production with two outgoing continuum positrons would be possible if no ground state e^- are present. Pair production, however, is suppressed by the Pauli principle if the ls levels are all full, so pre-ionization or stripping is necessary.

Müller et al.[7] have a given simple estimate for the positron production rate τ_+ in the collision of the two ions (see Fig. 3). The calculations are only done to lowest order in $Z-Z_{crit}$, and are similar to those made by Fano[9] in his discussion of the autoionization problem. The driving potential $\delta V = V - V_{crit}$ is proportional to $Z' = Z_1 + Z_2 - Z_{crit}$. Let $|\phi_c\rangle$ be the single particle solution of the Dirac equation

$$\mathscr{H}_0 |\phi_c\rangle \equiv \left[\vec{\alpha}\cdot\vec{p} + \beta m + V_{crit}\right] |\phi_c\rangle = -mc^2 \, |\phi_c\rangle$$

just at the critical value, and let $|\psi_E\rangle$ be the angular momentum zero, three-particle continuum state solution of

$$\mathscr{H}_0 |\psi_E\rangle = -E\, |\psi_E\rangle , \qquad E \leq -mc^2 \quad .$$

Then to first order in δV,

$$\epsilon_+ = mc^2 + \langle \phi_c | \delta V | \phi_c \rangle \sim mc^2 + Z' \delta , \qquad \delta = 29 \text{ keV}$$

$$\Gamma_+ \equiv \hbar/\tau_+ = 2\pi |\langle \psi_E | \delta V | \phi_c \rangle|^2 \sim Z'^2 \gamma , \qquad \gamma = 0.05 \text{ keV}$$

Clearly, we require that the distance R between the two ions be sufficiently small $R < R_{crit}$, and the collision overlap time T sufficiently large compared to τ_+ in order to satisfy the critical field strength condition and the adiabatic condition. An interesting discussion of the experimental conditions and the formation of superheavy quasi-molecules is given by Peitz, Müller, Rafelski and Greiner.[10] The above estimates are clearly only a guide: other corrections of order α from QED and the presence of the other atomic electrons need to be considered.

The observation of the production of electron-positron pairs via the coherent energy of the nuclear Coulomb field would clearly be a unique physical test of strong field quantum electrodynamics. However, the physics can be understood in terms of normal Feynman diagrams using bound state or Furry-picture quantum electrodynamics (see Fig. 4). We are clearly dealing with pair production arising from the collision of two charged particles: if the collision times are long enough, the produced e^- can bind to one of the nuclei and the outgoing positron will balance the overall linear and angular momentum. Clearly the energy to produce the continuum positron and bound electron comes from the kinetic energy of the colliding atoms. What is novel here is that the processes are occurring in a region where $Z\alpha > 1$, and normal perturbation theory is inapplicable. It may also be interesting to measure the photons which are internally produced during the collision.

Thus far, the most detailed check of quantum electrodynamics in the strong field regime is the comparison between theory and experiment for the K-electron binding energies in heavy atoms (W, Hg, Pb, Rn) (see Table I) and, most dramatically, in Fermium (see Table II). In particular, this astonishingly precise experimental[11] and theoretical work[12-17] already rules out nonlinear modification of QED of the type suggested by Born and Infeld[18] by two orders of magnitude. Notice also, that the QED effects due to the electron self-energy and vacuum polarization are being substantially checked in these comparisons. The situation is more clouded in the case of muonic atoms of large Z, since there are a few transitions [especially the 5g-4f transitions in ^{82}Pb and the 4f-3d transitions in ^{56}Ba] which show a 2σ disagreement between the most recent theoretical calculations and experiment. (See Table III.) A complete review has been given by Kroll.[19] The current status of Lamb shift measurements and theory for high Z elements has been reviewed by Erickson.[14]

There has been considerable theoretical interest in the question of whether the radiative corrections could modify or even eliminate the predictions discussed here for pair production at $Z > Z_{crit}$. As we have noted, the radiative corrections are controlled by α rather than $Z\alpha$ so they are in principle independently controllable in their physical effects, and thus one would not expect dramatic changes in the previous description. One also would not expect that calculations based on a Feynman diagram treatment indicated by Fig. 4, could be much affected by effects of order α.

In the case of the self-energy corrections to the electron line, a fraction α of the lepton charge is spread out over a Compton radius of the electron $\lambda\!\!\!^{-}_e$ [modulo a logarithmic tail out to the Born radius $1/mZ\alpha$ associated with the Bethe sum]. Such a distribution convoluted with the nuclear size distribution could only change Z_{crit} by a negligible amount.[20] Also, since the determination of the nuclear radius R derives from electron scattering experiments, the influence of radiative corrections is already partially included.

The situation is somewhat more complicated in the case of the vacuum polarization corrections, although in the end, the modifications turn out to be just as small. For small r ($r \ll \lambda\!\!\!^{-}_e$) the Serber-Uehling potential is of order

$$\frac{V_{vp}(r)}{V(r)} \sim \frac{2\alpha}{3\pi} \log \frac{1}{r\lambda\!\!\!^{-}_e} \quad ,$$

so that

$$\left\langle \frac{V_{vp}}{V} \right\rangle < \alpha \log \frac{1}{R\lambda\!\!\!^{-}_e} < 10^{-2}$$

for $R < 0.03\, \lambda\!\!\!^{-}_e$. In fact, Popov,[5] and also Peiper and Greiner,[4] find α_{crit} is changed in order 10^{-5}. The correction to the Serber-Uehling potential of the Wichman-Kroll type (from the Coulomb interactions of the electron-positron pair) is also incredibly small. The validity of an analytic expansion in $Z\alpha$ up to $(Z\alpha)_{crit}$ (and even beyond this value, where V_{vp} becomes complex) has been demonstrated by Popov.[5] Zeldovich and Gershtein, however, did raise the question of how important the "bound pair", discrete level contribution to the vacuum polarization loops might be. They argued that if the size of the bound-pair wavefunction increases, i.e., becomes delocalized, then it is conceivable that the vacuum polarization of this state might shield the physical electron from the effects of the critical field. However, as Popov[5] has shown, the radius of the state actually decreases! (See Fig. 5.) Popov's conclusion that vacuum polarization effects are negligible is supported by model calculations of Fulcher and Greiner[4] using a square-well potential. In Fulcher and Klein's work,[6] the nucleus in the correct vacuum state for $Z > Z_{crit}$ has an effective charge of Z-2 relative to the old vacuum. (This is also discussed in very general terms by A. Migdal.[23]) Thus there would be a change of order 2/Z in the vacuum polarization calculations. Accordingly, we can conclude that the higher order effects from quantum electrodynamics do not give anomalously large corrections to the critical field phenomena.[24]

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Wichmann-Kroll results to the case of finite nuclear size, claims the bound state with energy $\epsilon \sim -mc^2$ has an anomalously large vacuum polarization contribution of order $1/(Z-Z_{crit})$ due to its proximity to the negative energy continuum. In fact, the two contributions cancel when combined together and give a finite result.

TABLE I

K-Electron Binding Energies (in Ry)

from J. B. Mann and W. R. Johnson[12]

Element	Self-Energy and Vacuum Polarization*	E_{th}	E_{expt} (Ry)
W	8.65	-5110.50	-5100.46 ± .02
Hg	11.28	-6108.52	-6108.39 ± .06
Pb	12.27	-6468.79	-6468.67 ± .05
Rn	14.43	-7233.01	-7233.08 ± .90

*Calculated by A. M. Desiderio and W. R. Johnson. (See also G. Erickson.[14])

TABLE II

Binding Energies for Fermium (Z=100, A=254)

from B. Fricke, J. P. Desclaux, and J. T. Waber[15]

	1s	2s	$2p_{1/2}$
Electric	-142.929 keV	-27.734	-26.791
Magnetic	+ .715	+ .091	+ .153
Retardation	- .041	- .008	- .013
Vacuum Fluctuation (S.E.)	+ .457	+ .096	+ .009
Vacuum Polarization	- .155	- .026	- .004
Theoretical Total	-141.953 (26)	-27.581 (20)	-26.646 (10)
Experimental Value	-141.963 (13)	-27.573 (8)	-26.664 (7)

Theoretical Total -141.965 (25) from M. S. Freedman, F. T. Porter, and J. B. Mann.[16]

Born-Infeld correction[18]: 3.3 keV or 100 times Th-Exp.

TABLE III

Muonic Transition Energies in (eV) for the transitions $\alpha_1 = 4f_{5/2} - 3d_{3/2}$, $\alpha_2 = 4f_{7/2} - 3d_{5/2}$, $\beta_1 = 5g_{7/2} - 4f_{5/2}$, $\beta_2 = 5g_{9/2} - 4f_{7/2}$.

I	II	III	Vacuum Polarization of Order			VII	VIII	IX	X	XI	XII
$Z^{element}$ Transition	Point Nucleus Energy	Finite Size Effect	IV $\alpha(\alpha Z)$	V $\alpha^2(\alpha Z)$	VI $\alpha(Z\alpha)^3+$ $\alpha(Z\alpha)^5+$	Lamb Shift	Electron Screening	Nuclear Polarization	Order $\frac{v^2}{c^2}$ $\frac{m_\mu}{M_N}$	Energy (Theoretical)	Energy (Experimental)
$_{47}Ag$											
α_1	306970±2	-29±2	1519	10.5	-10.7	5±2	-12±1	5±2	1	308459±4	308428±19
α_2	303328±2	-11±1	1470	10.2	-10.4	-3±1	-12±1	4±1	1	304777±3	304759±17
$_{48}Cd$											
α_1	320422±2	-36±4	1608	11.2	-11.7	6±2	-13±1	5±2	2	321994±5	321973±18
α_2	316457±2	-14±2	1555	10.7	-11.4	-4±1	-13±1	4±1	1	317985±3	317977±17
$_{50}Sn$											
α_1	348233±2	-50±5	1795	12.5	-13.9	7±2	-13±1	6±2	2	349979±6	349953±20
α_2	343553±2	-19±2	1731	12.0	-13.5	-4±1	-13±1	5±2	2	345254±4	345226±18
$_{56}Ba$											
α_1	439068±2	-140±17	2435	17.0	-22.6	10±3	-17±2	9±3	3	441362±18	441299±21
α_2	431652±2	-53±6	2328	16.2	-21.9	-8±3	-17±2	8±3	3	433907±8	433829±19
β_1	200541±1	0	762	5.2	-9.5	2±1	-30±3	1±0	1	201273±3	201260±16
β_2	199193±1	0	748	5.1	-9.3	-1±0	-30±3	1±0	1	199908±3	199902±15
$_{82}Pb$											
β_1	435661±2	-10±1	2190	15.1	-51.2	8±0	-82±7	6±2	2	437739±8	437687±20
β_2	429343±2	-4	2106	14.5	-49.6	-7±0	-83±7	5±2	2	431327±8	431285±17

Reference: N. M. Kroll.[19]

FIGURE CAPTIONS

Figure 1: Energy eigenvalues as a function of nuclear charge. From L. P. Fulcher and W. Greiner, and W. Pieper and W. Greiner, Ref. 4.

Figure 2: Dependence of $(Z\alpha)_{crit}$ on the nuclear cutoff radius R. Here $\chi_e = \hbar/m_e c = 3.86 \times 10^{-11}$ cm. The asterisk indicates $Z_{crit} = 169$, $(Z\alpha)_{crit} = 1.25$ assuming $R = 1.1\ A^{\frac{1}{3}}$ f, $Z = 2.5\,A$ and a uniform distribution. From V. S. Popov, Ref. 5.

Figure 3: Dependence of the atomic energy levels on nuclear charge. The spreading of the positron escape width for the 1S level is shown as a function of $Z' = Z - Z_{crit}$.

Figure 4: Feynman diagram representation for positron production in ion-ion collisions. The produced electron becomes bound to the nucleus with charge $Z|e|$.

Figure 5: The mean radius $\bar{r}$ of the ground state as a function of its energy ϵ. The radius contracts to $\bar{r} = 0.31\ \chi_e$ at $\epsilon = -mc^2$, $(Z\alpha)_{crit} = 1.25$. From V. S. Popov, Ref. 5.

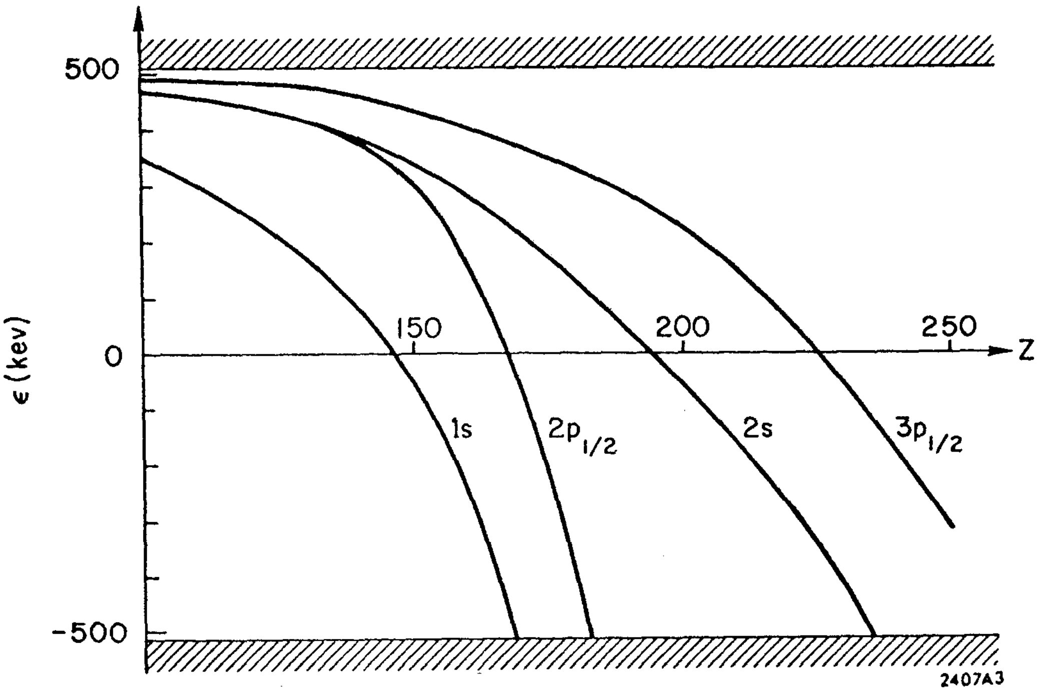
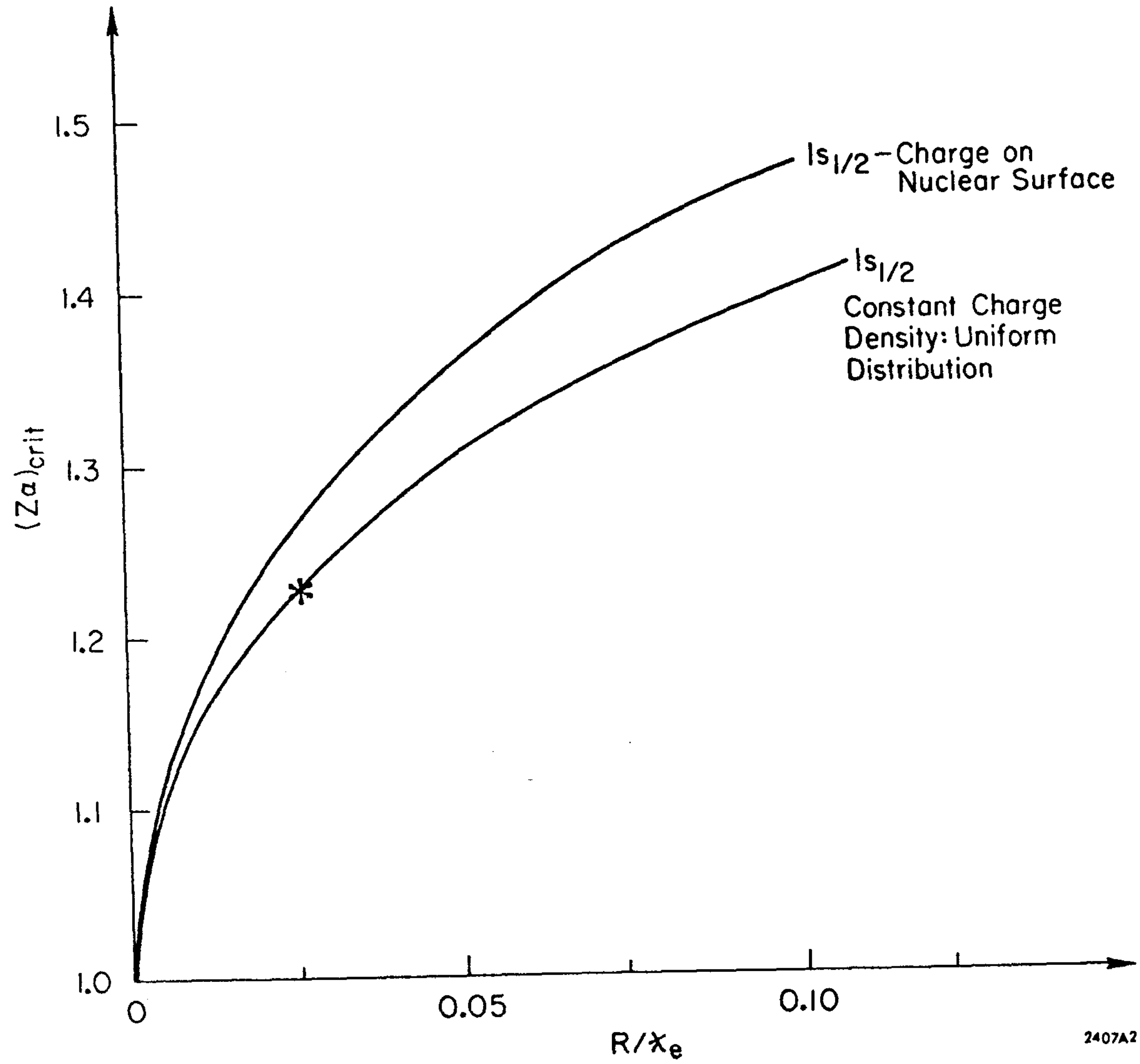


Fig. 1



1.5
1.4
1.3
1.2
1.1
1.0
$(Z\alpha)_{crit}$
$1s_{1/2}$ – Charge on Nuclear Surface
$1s_{1/2}$
Constant Charge Density: Uniform Distribution
0
0.05
0.10
R/λ_e
2407A2

Fig. 2

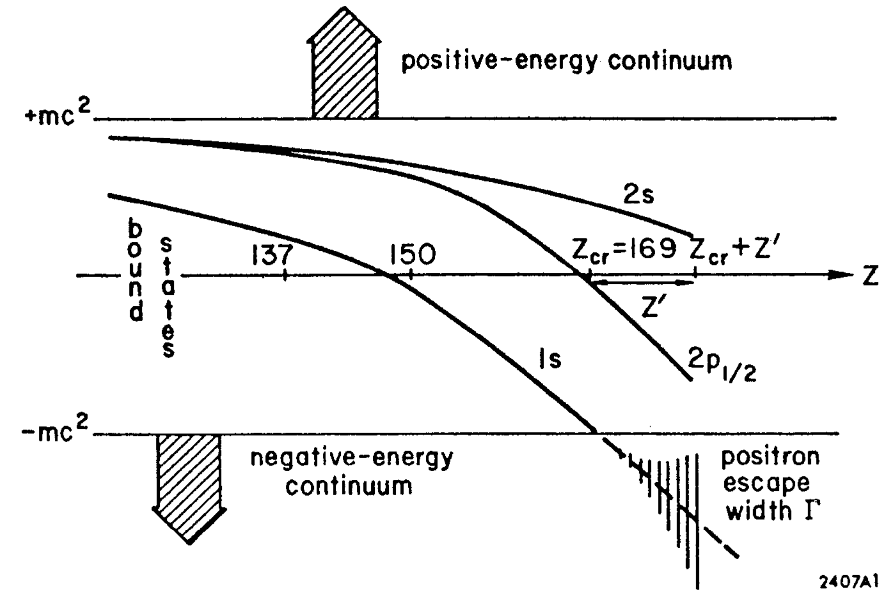

positive-energy continuum
+mc²
2s
bound states
137
150
Zcr=169
Zcr+Z′
Z
Z′
1s
2p1/2
-mc²
negative-energy continuum
positron escape width Γ
2407A1

Fig. 3

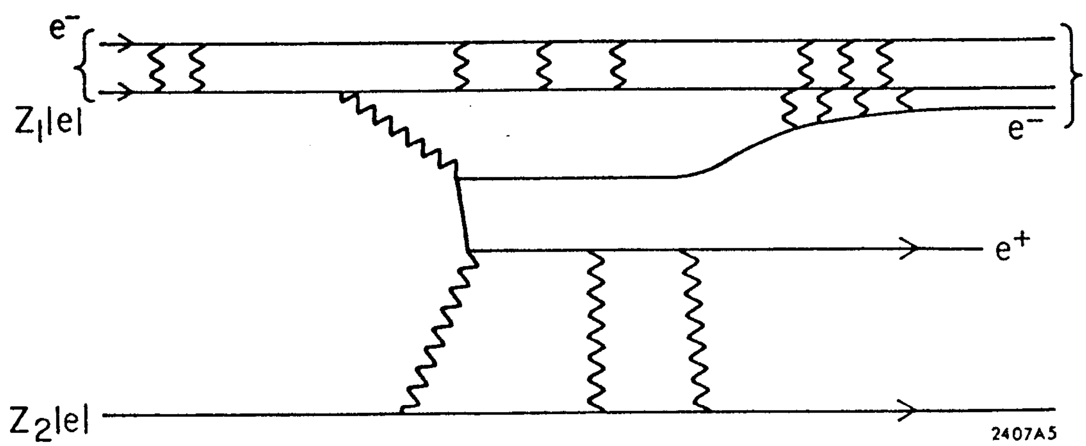

e⁻
Z1|e|
e⁻
e⁺
Z2|e|
2407A5

Fig. 4

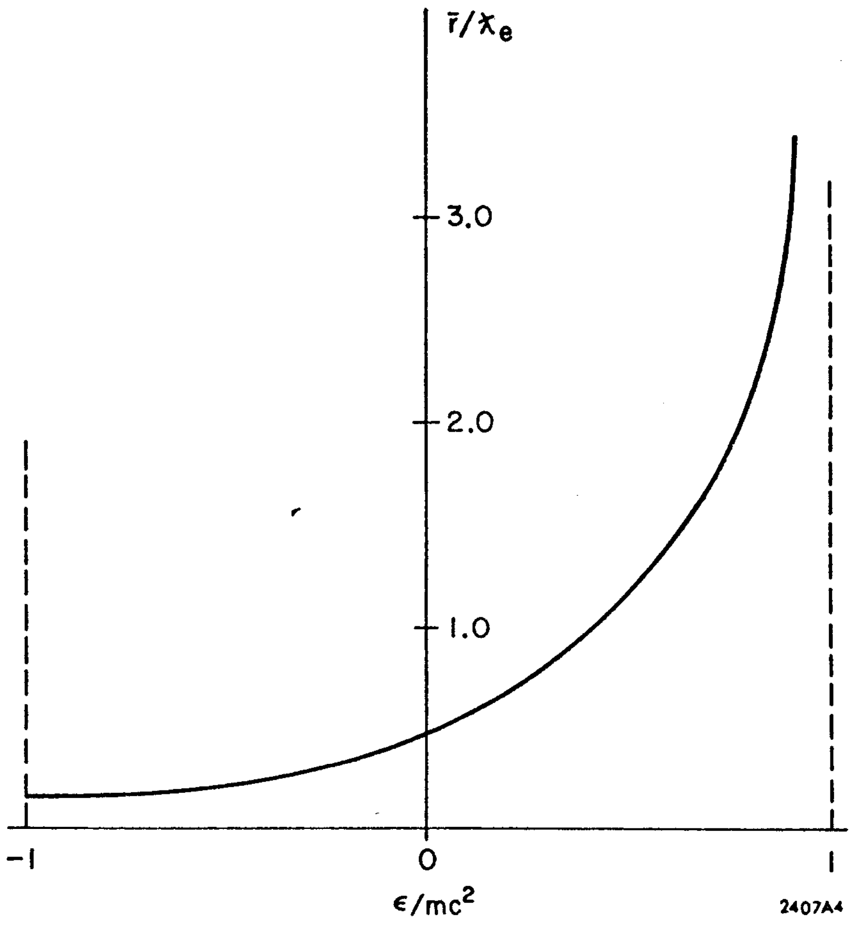


Fig. 5