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THREshold LAW FOR DOUBLE IONIZATION BY POSITRONS

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Threshold behaviour of the one-positron triple escape function has been studied within the classical theory. The ionization function energy dependence exponents $\varkappa$ are derived for a number of charges Z of residual ions: 2.966 ($Z = 1$), 3.604 ($Z = 2$), 4.011 ($Z = 3$), etc. Also, the possibility for an experimental verification of the results obtained analytically is discussed.

1. Introduction

Now as reasonably intensive low-energy positron beams are available[1], experimental study of the positron-atom (molecule) collisions has become feasible. A number of experiments with processes in which an impact positron participates have been already carried out, while other are planned and it is to be expected that a great deal of experiments done with electrons will be repeated with positrons. Up to now, however, only elastic processes with positrons have been investigated[2].

The rapid development of the experimental technique and the resulting increase of the experimental data has greatly stimulated theoretical investigations of the positron-atom collisions[2,3]. Similar to the experimental situation, only elastic processes calculations have been reported up to now. Generally, on the one hand, positron-atom collisions are easier to treat theoretically because of the absence of the exchange with the target electrons. On the other hand, the situation is more complicated here, due to the virtual or real positronium formations. These two features mutually compensate and the positron-atom scattering theory levels in difficulties with the corresponding methods designed for the electron scattering.

In the case of an ionization near the threshold, neither of the two effects plays a prominent role, since the particles in the final states are well separated, so as to be able to achieve free states in the asymptotic region[4]. Moreover, because of the dominance of the quasiasymptotic region in providing an ionization threshold law[5], the classical dynamics is applicable, and provides as reliable results as the semiclassical theory[6].

In Ref. 4 a method, based on the approach due to Vinkalns and Gailitis[7] has been developed, for the general case of an ionization of atom by a charged particle, and applied successfully to the case of the positron-atom collisions. The threshold law for the single ionization by positron has been thus derived and the results are in perfect agreement with the corresponding semiclassical calculations[6]. The method has been also extended to the case of double ionization by electrons[8], and the threshold law obtained agrees fully with earlier semiclassical data[9], confirming further the adequacy of the classical model in describing the threshold behaviour in atomic processes.

Here we present results of calculations for double ionization by the positron impact, making use of the same method, as described earlier. The extension from single to double ionization, however, turned out not to be trivial one, and the resulting formalism appears to comprise the essential features of both methods used in Ref. 4 and 8, respectively.

2. *One-positron triple escape*

As usually, derivation of threshold behaviour is carried out in several steps (cf. corresponding procedures in Refs. 4 and 8).

2.1. *The leading configuration*

In the zero-energy limit the escaping trajectories reduce to a set of zero measure in the total phase space. Among these ionizational configurations there exists a subset which possesses maximum symmetry, the type of which being determined by the kind of the escaping particles. As shown by Wannier[5] the outgoing particles move along a potential ridge, formed over the hyperplane $(\Phi\ 0\ \alpha)$ where Φ is the mutual angle and $\alpha = \operatorname{arc\,tg}(r_2/r_1)$ is the mock angle. When more than two particles are present, situation is more complicated, but the general property of the potential hypersurface remains: the system, at constant hyperradius R is stable with respect to the equilibrium mutual angles, and unstable regarding the mock angles (the saddle-point properties).

In the case of two electrons and one positron, moving in the field of a heavy ion with charge Z (atomic units are used throughout), the system is determined by 9 coordinates: $\vec{r}_1$ (first electron), $\vec{r}_2$ (second electron) and $\vec{r}_3$ (positron), with the residual ion at the origin. On the basis of motion in the asymptotic limit ($r_i \to \infty$, $i = 1, 2, 3$), at E (total energy) $= 0$, it can be easily shown that relevant final configurations are restricted to a fixed plane. Further, we chose Oz axis to coincide with the final positron velocity: $\dot{\vec{r}}_3 = \dot{r}_3 \hat{k}$, $t \to \infty$. Then the common plane will contain Oz axis, and we use the following system coordinates:

$$\begin{aligned}
&\text{first electron:} && r_1, \alpha_1 = \operatorname{arc\,tg}(r_1/r),\ \Phi_1 = \sphericalangle(\vec{r_1}, \hat{k}) \\
&\text{second electron:} && r_2, \alpha_2 = \operatorname{arc\,tg}(r_2/r),\ \Phi_2 = \sphericalangle(\vec{r_2}, \hat{k}) \\
&\text{positron:} && r_3, \alpha_3 = \operatorname{arc\,tg}(r_3/r),\ \Phi_3 = \sphericalangle(\vec{r_3}, \hat{k})
\end{aligned} \tag{1}$$

$R = [r_1^2 + r_2^2 + r_3^2]^{1/2} = r\sqrt{3},\ (\dot{r} > 0).$

We define so called correlation parameters (see Ref. 4)

$$\beta_i = \lim_{t\to\infty}(r_i/r),\ i = 1, 2, 3 \tag{2}$$

$$\Theta_i = \lim_{t\to\infty}\Phi_i,\quad i = 1, 2, 3,\quad (\Theta_3 = 0). \tag{3}$$

Hence, in the asymptotic region the potential can be taken as

$$V = V(R, \beta_2, \beta_3, \Theta_1, \Theta_2). \tag{4}$$

The correlation parameters are then determined by the stationarity conditions

$$\frac{\partial V}{\partial \beta_{i+1}} = 0,\quad \frac{\partial V}{\partial \Theta_i} = 0,\quad i = 1, 2 \tag{5}$$

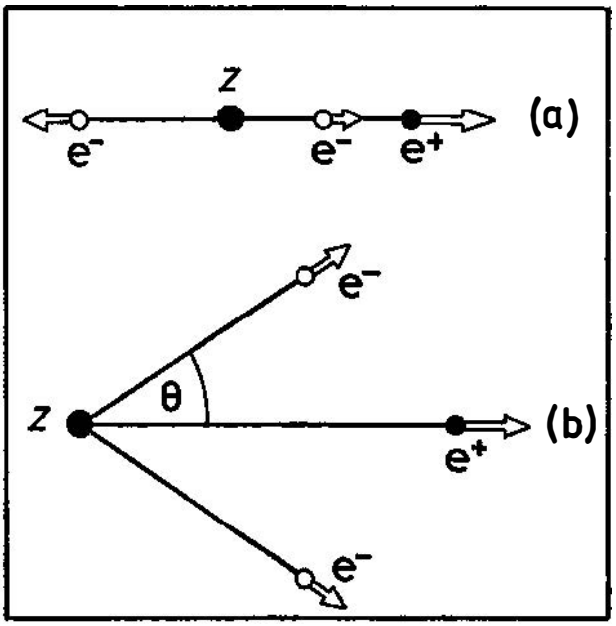
on the hypersphere: $R = \text{const}$. Even without writing explicitly right-hand side of Eq. (4), it is obvious that for the case at hand analytical solutions of Eqs. (5) are out of question, and even numerical calculations would be very tedious. Fortunately, we can simplify the problem on the physical grounds and single out those configurations, which appear realistic candidates for the leading trajectories. The resulting choice has been shown in Fig. 1. Case (a) corresponds to the choice

$$\Theta_1 = \pi,\quad \Theta_2 = 0\quad \text{(linear configuration)} \tag{6}$$

while (b) configuration is determined by

$$\beta_1 = 1,\quad \Theta_1 = \Theta_2 = \Theta. \tag{7}$$

However, even with these simplifications, it is not possible to find out analytical solutions, but numerical calculations of the potential V reveal the existence of a saddle point for the case (a). Numerical results for several Z-values are shown in Table 1. It is easy to show that the stationary points with respect to β_2, β_3 variables are maxima, whereas any displacement from the line (lateral displacement) creates a restitution force, i. e. corresponds to the potential minimum. A thorough numerical search for analogous stationary points within configuration (b) demonstrated nonexistence of the latters, though the shape of the potential function did suggest such a possibility, as evident from Fig. 2. Obviously, (b) configuration goes over to case (a) even if initially particles do form (b) - like structure. We hence procede with the linear asymptotic configuration.



.Fig. 1. Two possible candidates for the leading configurations in an one-positron triple escape

2.2. *Correlation parameters*

Let us write the longitudinal Δ_l and the transversal δ_l, ∇_l deviations in the form of column vectors

$$\vec{\Delta} = \begin{Bmatrix} \Delta_1 \\ \Delta_2 \\ \Delta_3 \end{Bmatrix}, \quad \vec{\delta} = \begin{Bmatrix} \delta_1 \\ \delta_2 \\ \delta_3 \end{Bmatrix}, \vec{\nabla} = \begin{Bmatrix} \nabla_1 \\ \nabla_2 \\ \nabla_3 \end{Bmatrix} \tag{8}$$

and let β_l be the components of a row vector

$$\vec{\beta} = \{\beta_1, \beta_2, \beta_3\}. \tag{9}$$

Further, we shall consider, without loss of generality, that the total angular momentum of the system is zero (see Ref. 4). Then, within the linear approximation one has

$$\vec{\beta} \cdot \vec{\delta} = 0, \ \vec{\beta} \cdot \vec{\nabla} = 0. \tag{10}$$

From the condition: $R = \text{const.}$ we obtain third equation

$$\vec{\beta} \cdot \vec{\Delta} = 0 \quad \text{(constant hypersphere)}. \tag{11}$$

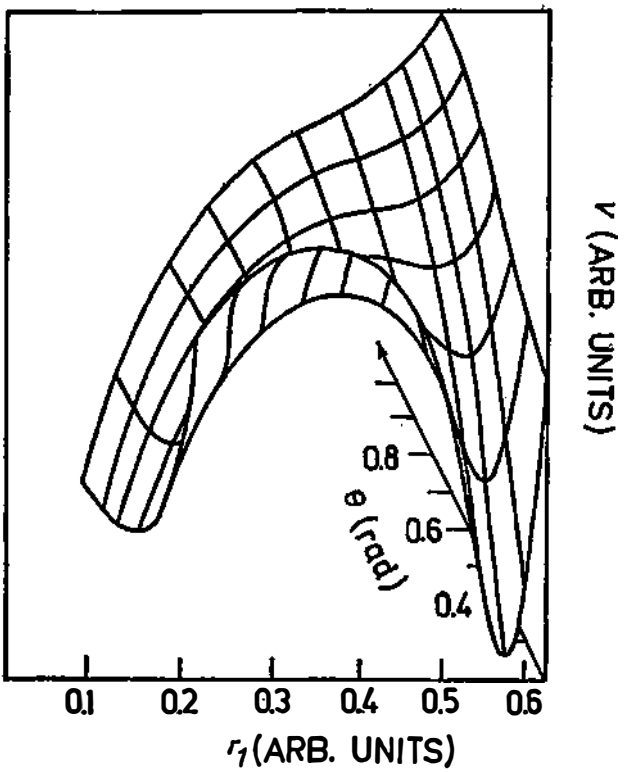


Fig. 2. Potential surface on the hypersphere R = const. for case (b) in Fig. 1.

2.3. *Derivation of the final-state trajectories*

Let the outgoing particles are charges $q_i, i = 1, 2, 3$, with unit masses, $m_i = 1, i = 1, 2, 3$. Then outside the innermost zone around the ion Z (where the quantum character of the system is essential), we assume that the classical dynamics holds[5], and the motion is governed by Newton's dynamics

$$\frac{\mathrm{d}^2 \vec{r}_i}{\mathrm{d}t^2} = Z \frac{q_i}{r_i^3} \vec{r}_i + q_i \sum_{j \neq i} \frac{q_j (\vec{r}_i - \vec{r}_j)}{|\vec{r}_i - \vec{r}_j|^3}, \quad i = 1, 2, 3. \tag{12}$$

We are interested in paths which cluster around the leading trajectories[4]

$$\vec{r}_i = \beta_i r \hat{k} + \Delta_i \hat{k} + \delta_i \hat{i} + \nabla_i \hat{j}, \quad i = 1, 2, 3 \tag{13}$$

with conditions

$$\Delta_i, \delta_i, \nabla_i \ll \beta_i r, \quad i = 1, 2, 3. \tag{14}$$

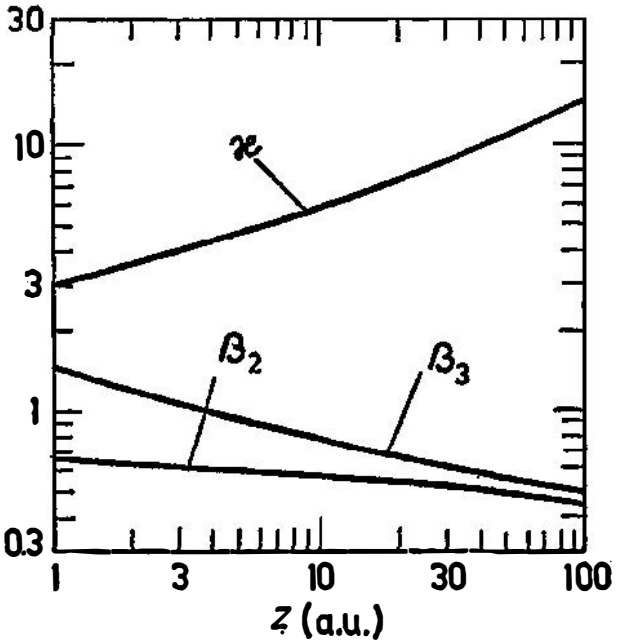


Fig. 3. Correlation parameters β (see text) and the threshold law exponent $\varkappa$ for one-positron triple escape, as function of the residual charge Z.

Inserting Eqs. (13) into Eq. (12) and retaining terms up to Δ_i/r, δ_i/r, ∇_i/r (linear approximation), one arrives (having accounted for the condition (11)) at the matrix equations

$$-\frac{r^3}{2}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\begin{Bmatrix}\Delta_1\\ \Delta_2\end{Bmatrix} = A\begin{Bmatrix}\Delta_1\\ \Delta_2\end{Bmatrix}, \quad A = \begin{Bmatrix}a_{11} & a_{12}\\ a_{21} & a_{22}\end{Bmatrix} \tag{15}$$

$$a_{11} = q_1\left[\frac{Z}{|\beta_1|^3} + \frac{q_2}{|\beta_1-\beta_2|^3} + \frac{q_3}{|\beta_1-\beta_3|^3} + \frac{\beta_1 q_3}{|\beta_3|\,|\beta_1-\beta_3|^3}\right]$$

$$a_{12} = q_1\left[\frac{\beta_2 q_3}{\beta_3\,|\beta_1-\beta_3|^3} - \frac{q_2}{|\beta_1-\beta_2|^3}\right] \tag{16}$$

$$a_{21} = q_2\left[\frac{\beta_1 q_3}{\beta_3\,|\beta_2-\beta_3|^3} - \frac{q_1}{|\beta_1-\beta_2|^3}\right]$$

$$a_{22} = q_2\left[\frac{Z}{|\beta_2|^3} + \frac{q_1}{|\beta_1-\beta_2|^3} + \frac{q_3}{|\beta_2-\beta_3|^3} + \frac{\beta_2 q_3}{|\beta_3|\,|\beta_2-\beta_3|^3}\right].$$

In deriving Eqs. (15) we have used equations for the unperturbed motion (all $\Delta_l, \delta_l, \Delta_l$ equal zero)

$$r^2 \frac{\mathrm{d}^2 r}{\mathrm{d}t^2} + b^2 = 0 \tag{17}$$

$$b^2 = q_1 \left[\frac{Z}{|\beta_1|^3} + \frac{q_2}{\beta_1 (\beta_1 - \beta_2)^2} + \frac{q_3}{\beta_1 (\beta_1 - \beta_3)^2} \right]. \tag{18}$$

If the energy of, say, first particle is E_1, then in the region where

$$E_1 r \ll b^2/|\beta_1| \text{ (note that all } E_l \text{ must be positive)}$$

one has an approximate solution of Eq. (17) (cf. Ref. 7)

$$r^3 \approx \frac{9}{2} b^2 t^2. \tag{19}$$

Obviously, relation (19) provides one-to-one correspondence between t and r, and may be used to take r as an independent variable in Eq. (15), which we cast into the form

$$-\left(\frac{3bt}{2}\right)^2 \frac{\mathrm{d}^2 \vec{\Delta}_{12}}{\mathrm{d}t^2} = A \vec{\Delta}_{12} \tag{20}$$

with obvious notation (cf. the first of Eqs. (8)). In the same way we obtain

$$2\left(\frac{3bt}{2}\right)^2 \frac{d^2 \vec{\delta}_{12}}{\mathrm{d}t^2} = A \vec{\delta}_{12}. \tag{21}$$

Equations of the type

$$gt^2 \frac{\mathrm{d}^2 \vec{F}}{\mathrm{d}t^2} = A \vec{F} \tag{22}$$

can be solved approximately by quasidiagonalizing matrix A. As this procedure has been described elsewhere (see Ref. 8, and references therein), we shall here only quote the result

$$\begin{Bmatrix} F_1 \\ F_2 \end{Bmatrix} = T \begin{Bmatrix} C_1 r^{\varkappa_1} + C_2 r^{\varkappa_2} \\ C_3 r^{\varkappa_3} + C_1 r^{\varkappa_4} \end{Bmatrix} \tag{23}$$

with C_l arbitrary constants, and with the exponents

$$\varkappa_{1,2} = \frac{3}{4}(1 \pm \sqrt{1 + 4u_1/g}) \tag{24}$$

$$\varkappa_{3,4} = \frac{3}{4}(1 \pm \sqrt{1 + 4u_2/g}) \tag{25}$$

where $u_{1,2}$ are the roots of the secular equation for A

$$u_{1,2} = \frac{1}{2}\{a_{11} + a_{22} \pm \sqrt{(a_{11} - a_{22})^2 + 4a_{12}\,a_{21}}\}. \tag{26}$$

As already mentioned, matrix T diagonalizes A only approximately. Note that A is non-hermitian and therefore T need not be unitary.

Because of the axial symmetry of the system, deviations δ_l and ∇_l appear completely equivalent, and everything said for the first is valid for the latter, too. Hence, by substituting values for g from Eqs. (20) and (21), one has solutions for Δ_l, δ_l, and ∇_l in the form of Eqs. (23). In Table 1 numerical values for $\varkappa_{1,3}$ expo-

TABLE 1.

Z	$\varkappa_1^{(0)}$	$\varkappa_1$	$\varkappa_3^{(0)}$	$\varkappa_3$
1	1.8575	1.8755	3.0994	3.0908
2	1.9283	1.9465	3.6647	3.6573
3	1.9523	1.9683	4.0490	4.0431
10	1.9844	1.9338	5.8150	5.8127
100	1.9973	1.9997	14.859	14.859

Numerical values for the exponents (see text).

nents are shown for several Z-values. $\varkappa_{2,4}$ can be deduced *via* Eqs. (24), (25). Also, we show in Table 1 zero-order $\varkappa_{1,3}^{(0)}$ values, which are obtained by setting $a_{12} = a_{21} = 0$ in A matrix. As can be seen, these values differ only insignificantly from the exact ones. For the same reason T appears almost unitary, but departure from the strict unitarity increases with Z, as it is evident from Table 2. In the

TABLE 2.

Z	T_{11}	T_{12}	T_{21}	T_{22}	$\lvert\Delta_{21}\rvert/\lvert\Delta_{11}\rvert$
1	0.98193	0.049998	0.18926	0.99880	0.006
2	0.94902	0.018344	0.31521	0.99983	0.018
3	0.92709	0.010198	0.37483	0.99995	0.032
10	0.8544	0.000	0.51954	1.000	0.105
100	0.701	0.000	0.713	1.000	0.441

The transformation matrix elements.

last column of the same table the ratio of modulus of largest off-diagonal element to modulus of smallest diagonal of the *diagonalized*, Λ matrix is shown, too.

2.4. *The threshold law*

How the threshold behaviour of the ionization cross section is derived from the trajectory equations in the form (23) has been shown elsewhere (see Ref. 4, and references therein). Here we outline the principal steps only. To fix the idea, we write the solution for $Z = 2$, with corresponding numerical values

$$\Delta_1 = 0.949\,(C_1\, r^{1.946} + C_2\, r^{-0.446}) + 0.02\,(C_3\, r^{3.657} + C_4\, r^{-2.157}) \tag{27}$$

$$\Delta_2 = 0.315\,(C_1\, r^{1.946} + C_2\, r^{-0.446}) + 0.9998\,(C_3\, r^{3.657} + C_4\, r^{-2.157}). \tag{28}$$

Analogous expressions can be written for δ_1, δ_2, but we do not need them here, since the deviations perpendicular to the leading trajectories are not important for this kind of triple escape. The crucial quantities are Δ_1/r, Δ_2/r, at large r, more precisely at $r = R_w$ (Wannier's radius), where the true asymptotic zone begins. If $R_w (\sim 1/E)$ is not taken too large that the second term in Eq. (27) becomes dominant, then between the Coulomb zone and the free motion region one has

$$\Delta_1/r \sim C_1\, r^{0.946}. \tag{29}$$

Similarly,

$$\Delta_2/r \sim C_3\, r^{2.657}. \tag{30}$$

Now, under a homothetic (shape preserving) transformation: $r \to r/E$, $\Delta r \to \Delta r/E$, left-hand side of Eqs. (29) — (30) are unaltered, whereas for the right-hand sides of the same equations it is ensured if

$$C_1 \sim E^{0.946}, \quad C_3 \sim E^{2.657}. \tag{31}$$

If particle *1* (electron) and particle *2* (positron) are to run away to infinity, by entering the free zone, Δ_i/r must be sufficiently small (i. e. trajectories should be reasonably close to the leading ones). However, there must exist C_1^{max} and C_3^{max} which still allow for the escapes of corresponding particles. These limiting values scale also according to Eqs. (31), so that the probability the first electron to run away behaves as

$$P_1 \sim E^{0.946}. \tag{32}$$

This can be compared with the corresponding probability for the case when the third particle (positron) is absent (original Wannier's case), when one has the law: $E^{1.056}$ (see Ref. 5), what at the same time determines the threshold law for double escape for $Z = 2$. Similarly, probability the second electron to reach the free zone is

$$P_2 \sim E^{2.657}. \tag{33}$$

It is to be compared with the probability for the escape in the absence of the first electron (see Ref. 4, and references therein), which is given by: $E^{2.9736}$ (single ionization by the positron impact). The joint probability for both electrons to reach the free zone is then the product of P_1 and P_2. By the relation (11), which states that if Δ_1/r and Δ_2/r are sufficiently small, so will be Δ_3/r, we arrive finally at the total probability for triple escape for $Z = 2$

$$\sigma_{ion} \sim P_1 \cdot P_2 \sim E^{\varkappa}, \; \varkappa = \varkappa_1 + \varkappa_3 - 2 = 3.604. \tag{34}$$

In the same manner one gets for $Z = 1$: $\varkappa = 2.966$, for $Z = 3$: $\varkappa = 4.011$, etc.

As can be inferred from Table 1, exponents determining the threshold laws increase with Z, analogously with the single ionization by positron (see Ref. 4). One encounters quite an opposite situation in the case of ionization by electrons, when an exponent for n-fold ionization decreases to n, in the limit $Z \to \infty$. This can be explained by the crucial role of the interparticle correlations in the small--energy region: for the symmetrical final configurations of identical particles, the role of the Coulomb field of the remaining ion becomes dominant with an increase of Z, the outgoing particles being well separated from each other. On the contrary, mutual distance between the second electron and positron diminishes in the limit $Z \to \infty$ and the correlation gains its importance. For the same reason it is not possible to obtain an asymptotic expression for β_2, β_3 (and thus for $\varkappa_i$) for large Z, analytically, since terms of the form: $1/(z_3 - z_2)$, or $1/(\beta_2 - \beta_3)$, must be treated on equal footing with those containing Z (e. g. Z/β_3, etc.) Nevertheless, one can infer from Table 1 that

$$\lim_{Z \to \infty} \varkappa_1 = 2$$

in accordance with above comparison with the single-ionization by electrons.

3. *Discussion and concluding remarks*

The present calculations provide for the first time threshold law for double ionization by positrons. In this sense, they represent the first classical result, after original Wannier's paper (1953), on the near-threshold ionization when there are neither experimental nor other theoretical results available. Having been tested on the positron-impact ionization (Ref. 4) and on triple electron escape (Ref. 8), the generalized Vinkalns-Gailitis classical method has proved highly successful in dealing with near-threshold processes, which at present are out of reach of the semiclassical theory and difficult to measure experimentally. Besides, the physical transparency of the method makes it a prospective tool for investigating other, more complicated processes, like the triple ionization by electrons (to be published elsewhere), etc.

As for the possible experimental verification of the present results, though at present hardly feasible, this can be done, in principle, *via* the proccesses of the type:

$$e^+ + He \rightarrow He^{2+} + 2e^- + e^+ \qquad (a)$$

$$[He; e^+] + h\nu \rightarrow He^{2+} + 2e^- + e^+ \qquad (b)$$

$$e^- + [He; e^+] \rightarrow He^+ + 2e^- + e^+ \qquad (c)$$

where $[He; e^+]$ denotes the one-positron (helium) atom. However, since one--positron systems seem to be unstable with respect to the positronium detachment[10], a process of type (a) is most probable to be investigated first. In fact, the positronium formation interferes with the near-threshold ionization of (a) type, as found by a numerical analysis of the single ionization by positrons[11], effecting particularly the energy distribution. In the case of double ionization, even more complicated situation is to be expected, at least as far as the energy partition is concerned. On the other hand, the infinite ion mass assumption, implicit in all analytical calculations (but see Ref. 12), is surely less crucial in the case of double ionization, than for the single one, since in the first case the final configuration appears more symmetrical than in the latter. In the light of failure to provide the threshold law for the electron-impact double ionization[13], it seems unlikely that the classical trajectory method could be used as a substitute for eventual experimental investigations, mentioned above.

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References

1) T. C. Griffith, Adv. Atom. Molec. Phys. **15** (1979) 135;

2) A. S. Ghosh, N. C. Sil and P. Mandal, Physics Reports **87** No 7 (1982) 313;

3) J. W. Humberston, Adv. Atom. Molec. Phys. **15** (1979) 101;

4) P. Grujić, J. Phys. **B 15** (1982) 1913;

5) G. H. Wannier, Phys. Rev. **90** (1953) 817;

6) H. Klar, J. Phys. **B 14** (1981) 4165;

7) I. Vinkalns and M. Gailitis, Latvian Academy of Science Report No 4 (Riga: Zinatne) (1967) 17;

8) P. Grujić, J. Phys. **B**, to be published;

9) H. Klar and W. Schlecht, J. Phys. **B 9** (1976) 1699;

10) D. C. Clary, J. Phys. **B 9** (1976) 3115;

11) M. S. Dimitrijević and P. Grujić, J. Phys. **B 16** (1983) 297;

12) H. Klar, Z. Phys. A-Atoms and Nuclei **307** (1982) 75;

13) M. S. Dimitrijević and P. Grujić, J. Phys. **B** 14 (1981) 1663.

ZAKON PRAGA ZA DVOSTRUKU JONIZACIJU POZITRONIMA

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Originalni naučni rad

Ponašanje funkcije jednopozitronskog trostrukog izletanja ispitivano je u okviru klasične teorije. Izračunati su eksponenti za energetsku zavisnost jonizacione funkcije za izvestan broj vrednosti naelektrisanja Z jonskog ostatka: 2.966 ($Z = 1$), 3.604 ($Z = 2$), 4.011 ($Z = 3$), itd. Diskutovane su mogućnosti eksperimentalne provere dobijenih rezultata.