PHYSICAL REVIEW A, VOLUME 64, 022715

Threshold laws for four-particle fragmentation

V. N. Ostrovsky*
Y. A. Fock Institute of Physics, The University of St Petersburg, 198904 St. Petersburg, Russia
(Received 15 November 2000; published 17 July 2001)

Breakup of an atomic particle into several charged fragments can be achieved by multiple photoionization or by collision processes. The threshold behavior of fragmentation cross sections is generally described by power laws, $\sigma_{\mathrm{fr}}\sim E^{\mu}$, where E is the excess energy above the breakup threshold. We evaluate threshold indices μ for four-fragment breakup of a large number of systems not considered before. All the fragments have different charges and (finite) masses with only one restriction imposed to limit the choice of systems considered: it is presumed that two of the fragments represent identical particles. Some previously suggested threshold laws are revised.

DOI: 10.1103/PhysRevA.64.022715 PACS number(s): 32.80.Fb, 34.80.Dp, 34.80.Kw

I. INTRODUCTION

Processes with several (three or more) charged particles in the final state exhibit a particular threshold behavior with regard to the cross section, as inferred by the famous Wannier law for the $(2e+\text{charged core})$ system

$$\sigma_{\mathrm{fr}}\sim E^{\mu}, \tag{1}$$

where E is the energy excess above the fragmentation threshold. The primary task of the theory is an evaluation of the threshold index μ.

Multiple fragmentation, distinct from the Wannier [1] three-particle case, was considered in the pioneering work by Klar and Schlecht [2]. These authors analyzed the escape of three electrons from the charged core (see also the paper by Grujić [3]). Instead of a linear configuration of receding particles treated by Wannier, Klar and Schlecht suggested that the electrons fly apart being in the apexes of an equilateral triangle with the core sitting in the center. The high symmetry of this particular system was employed to simplify the treatment, as also in the case of four-electron escape considered later by Grujić [4]. The use of specific constructions somewhat veiled the general issues of the theory, which were not explored fully.

The necessity of formulating a general approach emerged when the positron-containing systems became accessible for detailed experimental study. In order to provide a theoretical basis, Poelstra *et al.* [5] considered the escape of two electrons and one positron from the charged core. However, the result obtained by these authors proved to be inconsistent with the universal approach developed later by Kuchiev and Ostrovsky [6] (see also the brief exposure in Ref. [7]). The main features of this general theory could be formulated as follows. The threshold law is governed by a *scaling configuration* of receding particles in classical mechanics. In such a configuration, by definition, the time evolution of all particle coordinates in the center-of-mass frame is confined to a scale transformation with the common time-dependent scaling factor (see Sec. II for more detail). No particular fragmentation coordinate could or should be introduced in a natural way. The scaling configuration is unstable, and its unstable modes produce partial threshold indices μ_j that sum up to the total index entering the threshold law (1),

$$\mu=\sum_j \mu_j . \tag{2}$$

Since the summation runs over all unstable modes, there are no unaccounted modes to justify the appearance of secondary threshold laws. The theory of near-threshold breakup is designed in a purely dynamic way and does not appeal to statistical arguments. From a more technical standpoint, the hyperspherical coordinates, which are useful in various few-body problems, do not provide noticable advantages when the threshold laws are concerned. Even more, use of these coordinates complicates the calculations unnecessarily.

These particular features of the approach developed by Kuchiev and Ostrovsky as compared with the schemes suggested by other authors were already discussed in Ref. [6]. Here we add only some remarks related to the most recent publications. The secondary threshold law for three-electron escape is ruled out by experiments [8]. The problem of the discrepancy between the results of Refs. [5] and [6] for double ionization of an ion by positron impact was resolved in a careful theoretical analysis by Bluhme *et al.* [9], who showed that treatment in Ref. [5] omits one of two unstable modes. It is now finally confirmed [7,10,11] that no logarithmic factors emerge to modify the form of the threshold law (1).

From an experimental standpoint, we refer to recent studies of three-electron photoionization [13,8] and double ionization by positron impact [12]. Although the near-threshold domain is notoriously difficult for experimental observation, clear interest in the threshold behavior of multiparticle breakup persists. This, along with a theoretical appeal, inspired the more detailed study of four-particle fragmentation undertaken below. Compared to previous research, the presence of infinitely massive particles in the system is not assumed. We presume that masses of all fragments are finite and thus fully account for the recoil effects. We include for consideration some particles exotic to atomic physics, such as mesons or antiprotons. In order to limit various possible

*Email address: Valentin.Ostrovsky@pobox.spbu.ru

combinations and retain the feasibility of experimental observation, we consider systems with two identical particles (that are usually electrons or protons). For the fragment charges, we consider both available possibilities: (i) two particles with positive charge and two particles with negative charge, and (ii) one particle with positive (negative) charge and three particles with negative (positive) charges.

II. SCALING CONFIGURATIONS

The general condition defining scaling configurations was thoroughly discussed by Kuchiev and Ostrovsky [6], where the reader can find proofs and details. Let $\vec{r}_j(t)$ be the position of the jth particle in the center-of-mass frame. In the scaling configuration, by definition, acceleration of each particle is proportional to its vector $\vec{r}_j$,

$$\frac{d^2\vec{r}_j}{dt^2} = -\alpha\vec{r}_j, \tag{3}$$

with a common j- and t-independent factor α. Then time evolution of the system is reduced to a uniform expansion of the configuration in space, which does not change its shape. It is easy to show that relation (3) holds provided it is ensured at some initial moment of time $t=t_0$:

$$\frac{1}{m_j}\vec{F}_j = -\alpha\vec{\rho}_j, \tag{4}$$

where $\vec{\rho}_j = \vec{r}_j(t_0)$. The Coulomb interaction between the particles is presupposed, which allows one to evaluate the force $\vec{F}_j$ acting at $t=t_0$ on the jth particle as

$$\vec{F}_j = \sum_{n\neq j} q_j q_n \frac{\vec{\rho}_j - \vec{\rho}_n}{|\vec{\rho}_j - \vec{\rho}_n|^3}, \tag{5}$$

where q_j is the jth particle charge. Substitution of this expression into Eq. (4) gives a set of equations,

$$\frac{q_j}{m_j}\sum_{n\neq j} q_n \frac{\vec{\rho}_j - \vec{\rho}_n}{|\vec{\rho}_j - \vec{\rho}_n|^3} = -\alpha\vec{\rho}_j, \tag{6}$$

that serves to define the essential (scaling invariant) parameters of the configuration. Now we consider the specific form of these general equations in the case of a four-particle system.

Let two identical particles 1 and 2 have the same mass m_1 and negative charge $e=-1$. The particle 0 is the "atomic nucleus" with mass m_0 and charge $Z>0$. The particle 3 has mass m_3 and charge $-Z_3$ (it could be negatively charged, for instance an electron $Z_3>0$, or positively charged, for instance a positron $Z_3<0$). It is worthwhile to remember that simultaneous scaling of all charges or all masses does not influence the threshold index.

In the case of four fragments, all the particles lie in the same plane [14] and the shape of the scaling configuration is defined by four angles. If two particles are identical, then the scaling configuration has a symmetry axis that joins two

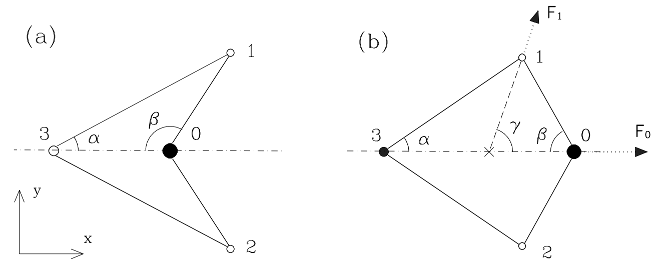

FIG. 1. Scaling configuration for four charged particles. Particles with negative/positive charges are shown by closed/open circles. Two identical particles are designated as 1 and 2. Plot (b) shows also the center-of-mass position ($\times$) and forces acting on the particles 1 and 0.

other particles. The scaling configuration is fixed by two angles α and β as shown in Fig. 1, where negatively (positively) charged particles are depicted by open (closed) circles. The cases $Z_3<0$ and $Z_3>0$ correspond to Figs. 1(a) and Figs. 1(b), respectively, which are described by the same equations derived below.

According to Eq. (4), the force $\vec{F}_j$ acting on each particle is directed along its vector $\vec{\rho}_j$ relative center of mass. For nonidentical particles 0 and 3, this condition follows automatically from symmetry. For the identical particles 1 and 2, it leads to a single equation, see Fig. 1(b),

$$\frac{F_{1y}}{F_{1x}} = \tan\gamma. \tag{7}$$

One more condition manifests the requirement (4) that for all the particles, the acceleration should be proportional to their coordinates $\vec{\rho}_j$ within a common scaling factor,

$$\frac{F_k}{F_j} = \frac{\rho_k m_k}{\rho_j m_j}. \tag{8}$$

The azimuthal angle γ of the particle 1 in the center-of-mass frame is readily expressed via α, β, and particle masses m_j. After substituting formulas (5) for Coulomb forces and some algebra, we obtain finally the set of two equations for the angles α and β fixing the scaling configuration,

$$\begin{aligned}(Z\sin^2\beta\cos\beta + Z_3\sin^2\alpha\cos\alpha)\sin\alpha\sin\beta \\ = \left(-Z\sin^3\beta + Z_3\sin^3\alpha + \frac{1}{4}\right)[\sin\alpha\cos\beta - \Xi_0(\alpha,\beta)],\end{aligned} \tag{9}$$

$$\begin{aligned}Z_3 m_1\left(Z\frac{\sin^2\beta}{\sin^2(\alpha+\beta)} - 2\cos\alpha\right)[\sin\alpha\cos\beta - \Xi_0(\alpha,\beta)] \\ = -m_3\left(Z\frac{\sin^2\beta\cos\beta}{\sin^2\alpha} + Z_3\cos\alpha\right)[\sin(\alpha+\beta) \\ + \Xi_0(\alpha,\beta)],\end{aligned} \tag{10}$$

where

TABLE I. Threshold indices for four-particle systems with three identical particles.

Fragments	μ	μ [15]
$H^+ + 3e^-$	2.8274	
$D^+ + 3e^-$	2.8268	
$^4He^{2+} + 3e^-$	2.2706	2.2706
$^{238}U^{2+} + 3e^-$	2.2704	2.2704
$^7Li^{3+} + 3e^-$	2.1621	2.1621
$^{238}U^{3+} + 3e^-$	2.1620	2.1620
$^9Be^{4+} + 3e^-$	2.1157	2.1157
$\mu^+ + 3e^-$	2.8367	
$e^+ + 3e^-$	4.2218	
$e^- + 3p^+$	113.86	

$$\Xi_0(\alpha,\beta)=\frac{2m_1\sin\alpha\cos\beta-m_3\sin(\alpha+\beta)}{2m_1+m_3+m_0}. \qquad (11)$$

The quantity $-\Xi_0/\sin\beta$ corresponds to ρ_{0x}, i.e., the x coordinate of the particle 0 with respect to the center of mass. Equation (9) follows from Eq. (7); Eq. (10) represents the specific form of Eq. (8) for $k=3,\ j=1$.

A special situation emerges for two pairs of identical particles. Due to symmetry reasons, the scaling configuration represents a rhombus fixed by a single angle. An equation for this parameter was deduced in Ref. [6].

For calculation of the threshold indices, one has to construct the matrix **V** of the potential second derivatives evaluated at the scaling configuration. The partial indices μ_j are directly expressed via eigenvalues of the matrix **KV**, where **K** is the matrix of particle inverse masses. All details can be found in Ref. [6].

III. THRESHOLD INDICES

A. Three identical particles and one particle of opposite charge

In this case, the scaling configuration is an equilateral triangle—$\alpha=30°,\beta=120°$—considered originally by Klar and Schlecht [2]; see the discussion in Sec. I. The threshold index is defined by the doubly degenerate unstable mode. The new element in our treatment of this old problem is taking into account the recoil effect, i.e., for finite mass of the central particle. Our results in Table I show that the threshold index μ increases as the mass of the central (positively charged) particle decreases. As anticipated, the isotopic effects are small in the case of an atomlike system, when the central particle is much more massive than three other particles. However, for $3e^-+e^+$ fragmentation, when all masses are equal, the value of the threshold index becomes much larger than in the atomlike situation. The "mass-inverted" case $3p+e^-$, with a light particle in the center of the triangle, exhibits a huge threshold index. Our results coincide with those published recently by Pattard and Rost [15] in cases in which the latter ones are available.

It is worthwhile to emphasize that the threshold index depends only on the system final state and not on its initial state. Therefore, generally we do not discuss the way in which the fragmentation is achieved; in some cases, more than one ingoing channel is possible; see Sec. III C. It should be noted that the ingoing channels look quite natural for atomic physics in all cases considered; for instance, $3e^-+e^+$ and $3p+e^-$ could be produced, respectively, by collisions $e+Ps^-$ and $H^++H_2{}^+$.

B. One positive and three negative charges

In variance with the previous case, here only two negatively charged particles are identical. The effect of the third

TABLE II. Parameters of scaling configuration (SC) and threshold indices for four-particle systems with a pair of identical particles. Between two other particles, one has a positive and the other a negative charge.

Fragments	SC parameters α	SC parameters β	μ_1	μ_2	μ	μ [15]
$H^+ + \mu^- + 2e^-$	43.69°	120.93°	2.5706	1.6680	4.2385	
$D^+ + \mu^- + 2e^-$	43.90°	120.79°	2.5923	1.6748	4.2671	
$H^+ + \pi^- + 2e^-$	44.19°	120.80°	2.7271	1.7323	4.4595	
$H^+ + p^- + 2e^-$	46.45°	120.09°	4.1272	2.3609	6.4881	
$D^+ + p^- + 2e^-$	46.82°	119.83°	4.5628	2.5632	7.1260	
$H^+ + \Sigma^- + 2e^-$	46.45°	120.09°	4.3014	2.4435	6.7449	
$^4He^{2+} + \mu^- + 2e^-$	52.77°	117.20°	1.1748	1.0550	2.2299	
$^4He^{2+} + \pi^- + 2e^-$	54.08°	116.53°	1.1735	1.0513	2.2248	
$^4He^{2+} + p^- + 2e^-$	61.55°	112.49°	1.1640	1.0320	2.1960	1.965
$^{238}U^{2+} + p^- + 2e^-$	65.06°	109.22°	1.1527	1.0245	2.1773	2.002
$^4He^{2+} + \Sigma^- + 2e^-$	62.17°	112.18°	1.1634	1.0307	2.1940	
$^7Li^{3+} + \mu^- + 2e^-$	54.52°	116.25°	1.0841	1.0253	2.1095	
$^7Li^{3+} + \pi^- + 2e^-$	55.90°	115.50°	1.0825	1.0231	2.1056	
$^3Li^{3+} + p^- + 2e^-$	63.50°	111.31°	1.0738	1.0128	2.0866	2.033
$^7Li^{3+} + \Sigma^- + 2e^-$	64.05°	111.08°	1.0733	1.0122	2.0856	

TABLE III. Parameters of scaling configuration (SC) and threshold indices for four-particle systems with a pair of identical particles. Two other particles have charges with the sign opposite to the charges of idential particles. The number in parentheses indicates the degree of unstable mode degeneracy.

Fragments	SC parameters α	SC parameters β	μ_1	μ_2	μ	μ [15]
$H^+ + e^+ + 2e^-$	27.61°	38.37°	1.8836	1.5613	3.4449	
$D^+ + e^+ + 2e^-$	27.60°	38.37°	1.8843	1.5618	3.4461	
$H^+ + \mu^+ + 2e^-$	29.99°	30.06°	22.533	16.759	39.291	
$H^+ + \pi^+ + 2e^-$	29.99°	30.04°	25.510	18.975	44.485	
$H^+ + H^+ + 2e^-$	29.998°	29.998°	50.330	37.462	87.492	
$D^+ + H^+ + 2e^-$	30.001°	30.006°	58.147	43.288	101.44	
$D^+ + D^+ + 2e^-$	29.9988°	29.9988°	71.251	53.052	124.30	
$H^+ + \Sigma^+ + 2e^-$	30.003°	30.005°	53.231	39.624	92.855	
$2e^+ + 2e^-$	45°	45°	1.2937	0.90584(2)	3.1053	
$^4He^{2+} + e^+ + 2e^-$	30.692°	27.587°	2.0447	1.7928	3.8375	3.764
$^{238}U^{2+} + e^+ + 2e^-$	30.69°	27.587°	2.0450	1.7931	3.8381	3.765
$^4He^{2+} + \mu^+ + 2e^-$	32.51°	21.24°	25.697	19.427	45.123	
$^4He^{2+} + \pi^+ + 2e^-$	32.52°	21.23°	29.430	22.249	51.678	
$^4He^{2+} + H^+ + 2e^-$	32.53°	21.20°	69.787	52.781	122.57	96.4
$^4He^{2+} + D^+ + 2e^-$	32.53°	21.20°	90.066	68.129	158.19	
$^{238}U^{2+} + H^+ + 2e^-$	32.53°	21.20°	77.956	58.965	136.92	107.4
$^4He^{2+} + \Sigma^+ + 2e^-$	32.53°	21.20°	76.519	57.876	134.40	
$^7Li^{3+} + e^+ + 2e^-$	32.09°	22.71°	2.2063	1.9719	4.1783	4.115
$^{238}U^{3+} + e^+ + 2e^-$	30.69°	27.59°	2.0450	1.7931	3.8381	3.765
$^7Li^{3+} + \mu^+ + 2e^-$	33.63°	17.42°	27.729	21.002	48.731	
$^3Li^{3+} + \pi^+ + 2e^-$	33.63°	17.41°	31.814	24.094	55.908	
$^7Li^{3+} + H^+ + 2e^-$	33.64°	17.39°	78.296	59.313	137.61	107.9
$^7Li^{3+} + \Sigma^+ + 2e^-$	33.64°	17.38°	86.680	65.667	152.35	

particle mass m_3 on the threshold index is not simple, as Table II shows [16]. When the positive charge Z is equal to unity, the threshold index μ increases with m_3. For larger Z, the opposite trend is observed. As discussed in Ref. [6], in the absence of particle correlation, the threshold index for the systems with one positive charge tends *from above* to the value $(N-2)$, i.e., 2 in the systems under consideration. Physically this limit is approached as the charge Z increases, in agreement with Table II. Moderately large values of threshold indices predicted for $Z=1$ probably could be eventually observed in experiments on fragmentation in collisions of p^- (or μ^-) with H^- or other negative ions.

There is an appreciable difference between our threshold indices and those reported by Pattard and Rost [15]. Their prediction of the threshold index below 2 in the case of $^4He^{2+} + p^- + 2e^-$ fragmentation products looks particularly challenging in view of the preceding discussion. A similar discrepancy occurs for the systems considered in Sec. III C. It is hardly possible to trace its origin since the method of calculations used in Ref. [15] is not specified. Our results gain support, in particular, from the useful and sensitive check provided by our scheme [6]. Namely, as mentioned in Sec. II, the partial threshold indices μ_j are expressed via eigenvalues of the matrix **KV**. This matrix has also other eigenvalues, and for some of them the explicit expressions via parameters of the scaling configuration are known. Any calculation error does not allow one to reproduce these *a priori* known eigenvalues.

C. Two positive and two negative charges

In the case of two positively charged particles, the threshold indices are generally larger than for a single positive charge; see Table III. The indices increase with Z, as discussed in Ref. [6]. Large isotopic effects are exemplified by comparison of systems $2H^+ + 2e, H^+ + D^+ + 2e$, and $2D^+ + 2e$; note that the shape of the scaling configuration exhibits very small variations. For fixed m_0, the threshold index μ increases with m_3.

The number of unstable modes (taking into account degeneracy) almost always equals $(N-2)$, i.e., 2 for four-body fragmentation. The rare exception is given by the $2e^+ + 2e^-$ system when one more unstable mode appears: this system has one nondegenerate and one doubly degenerate mode. Experiments for this unconventional situation would be very interesting, in part because there is some theoretical discussion on the subject; see Refs. [6,11]. Note that these fragments could be produced by positron-"ion" collision $e^+ + Ps^-$, or by "atom"-"atom" collision Ps+Ps, or by photofragmentation of the Ps_2 "molecule."

IV. CONCLUSION

The scaling configurations and threshold indices represent basic properties of few-body Coulomb systems. They characterize correlations in particle motion that are particularly strong in the near-threshold domain, where all the particles are slow and for a long time feel long-range Coulomb interaction. These fundamental characteristics are simple enough to evaluate by theory without any ambiguity, with any prescribed accuracy.

In the present paper, threshold indices are calculated for a number of four-particle fragmentation processes; the cases that are interesting from a theoretical point of view and feasible for experimental study are discussed. Experimental observation of threshold behavior is generally a difficult task, because near the threshold the cross section is low. The energy range where the threshold law is operative usually is not specified by standard threshold theories. Establishing this range is conventionally considered as a separate problem. The situations in which the threshold index is large are particularly difficult, implying detection of very weak signals in experiment. From this point of view, huge threshold indices are mostly of academic interest. Note, however, that Rost and Pattard [17] used with some success even very large threshold indices in constructing interpolation formulas for the cross sections useful in a broad energy range.

In molecular systems, the so-called adiabatic threshold is usually simply attainable. It corresponds to the ionization of molecules for space-fixed nuclei. The adiabatic threshold usually appreciably exceeds the energetic threshold to which the present discussion of threshold behavior applies. Below the adiabatic thresholds, the fragmentation cross sections are very small, which hinders experimental study. However, recently Bolognesi *et al.* [18] were able to observe fragmentation of an O_2 molecule into $O^+ + O^+$ ions below the adiabatic threshold.

Note added in proof. Recently we became aware that the first approach to the threshold law for double ionization of an atom by positron impact was done by P. Grujić [19].

[1] G. H. Wannier, Phys. Rev. **90**, 817 (1953).

[2] H. Klar and W. Schlecht, J. Phys. B **10**, 1699 (1976).

[3] P. Grujić, J. Phys. B **16**, 2567 (1983).

[4] P. Grujić, Phys. Lett. A **96**, 233 (1983); **122**, 494 (1987).

[5] K. A. Poelstra, J. M. Feagin, and H. Klar, J. Phys. B **27**, 781 (1994).

[6] M. Yu. Kuchiev and V. N. Ostrovsky, Phys. Rev. A **58**, 321 (1998).

[7] M. Yu. Kuchiev and V.N. Ostrovsky, J. Phys. IV **9**, 51 (1999).

[8] R. Wehlitz, T. Pattard, M.-T. Huang, I. A. Sellin, J. Burgdörfer, and Y. Azuma, Phys. Rev. A **61**, 030704 (2000).

[9] H. Bluhme, H. Knudsen, and J. P. Merrison, J. Phys. B **33**, 5463 (2000).

[10] M. Yu. Kuchiev and V. N. Ostrovsky, Phys. Rev. Lett. **85**, 4409 (2000).

[11] T. Pattard and J. M. Rost, Phys. Rev. Lett. **85**, 4410 (2000).

[12] H. Bluhme, H. Knudsen, J. P. Merrison, and M. R. Poulsen, Phys. Rev. Lett. **81**, 73 (1998).

[13] R. Wehlitz, M.-T. Huang, B. D. DePaola, J. C. Levin, I. A. Sellin, T. Nagata, J. W. Cooper, and Y. Azuma, Phys. Rev. Lett. **81**, 1813 (1998).

[14] In case (i), two positively and two negatively charged particles, the linear scaling configurations are also possible. However, these configurations lead to larger threshold indices than plane configurations and hence should be discarded as discussed in Ref. [6].

[15] T. Pattard and J. M. Rost, Phys. Scr. **T80**, 95 (1999).

[16] The masses used in the present calculations (in a.u.) are $m_\mu = 208.79$, $m_\pi = 273.13$, $m_{\Sigma^+} = 2327.5$, $m_{\Sigma^-} = 1192.47$.

[17] J. M. Rost and T. Pattard, Phys. Rev. A **55**, R5 (1997).

[18] P. Bolognesi, D. B. Thompson, L. Avaldi, M. A. MacDonald, M. C. A. Lopes, D. R. Cooper, and G. C. King, Phys. Rev. Lett. **82**, 2075 (1999).

[19] P. Grujić, Fizika (Zagreb) **15**, 213 (1983).