Threshold laws for the breakup of atomic particles into several charged fragments

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Processes with three or more charged particles in the final state exhibit a particular threshold behavior, as inferred by the famous Wannier law for a $(2e+\text{ion})$ system. We formulate a general solution which determines the threshold behavior of the cross section for multiple fragmentation. Applications to several systems of particular importance with three, four, and five leptons (electrons and positrons) in the field of a charged core, and two pairs of identical particles with opposite charges, are presented. Threshold exponents for these systems are predicted, while some previously suggested threshold laws are revised. [S1050-2947(98)04007-4]

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I. INTRODUCTION

The famous Wannier [1] threshold law has quite an unusual status among other threshold laws in quantum mechanics. Being based on an appealing mechanism, it has inspired a large number of studies where the law was rederived, extended, tested or rebutted. The intensity of these studies does not show a decrease with time, as shown in some recent publications [2–21]. A complete bibliography on the subject would be immense.

In this paper, we suggest a method which generalizes the Wannier mechanism when breakup of the quantum system on a *large number* (four or more) of charged fragments is concerned. Apparently, the particular case of the problem was treated for the first time in 1976 in an important paper by Klar and Schlecht [22], where the threshold law was derived for escape of three electrons from the charged core. It was suggested that the receding electrons form a symmetrical configuration of an equilateral triangle with a positively charged core in its center. The treatment was quite involving, and based on a hyperspherical coordinate system [23]. Later Grujić [24] rederived the same result using standard Cartesian coordinates, where the symmetry considerations are easy to apply explicitly to a full extent. Grujić also considered some other systems along the same lines [25–27] (see more details in Sec. V). The threshold law for the three-electron escape seems to find support in experimental data on the near-threshold double ionization of atoms by electron impact [28]. Later, Feagin and Filipczyk [29] claimed the existence of a complementary law which is manifested at energies somewhat above a threshold; see the critical discussion in Sec. V A.

Interest in the problem was renewed recently when two electrons and a positron receding from a core with $Z=1$ charge were considered in Ref. [30]. A brief note by Stevens and Feagin [31] on complete fragmentation of the H_2 molecule is also to be mentioned. The final state in the reaction with a positron could be produced by double ionization of a negative ion by positron impact. However, forthcoming experiments by Blohme, Knudsen, and Merrison [32] concern positron impact double ionization of neutral atoms $(Z=2)$, where the threshold law is not yet available. Its derivation was one of the motivations for the present study. Eventually it developed into a general approach to the multifragmentation problem which possesses two important advantages. First, our method describes a general situation with an arbitrary number of charged fragments in simple terms in an arbitrary coordinate frame. Second, it is convenient and reliable for practical realizations. This allows us to clarify important conceptual aspects of the problem which were misunderstood or misinterpreted previously. Comparing our solution with results in the literature, we reproduce a number of threshold exponents for different systems. At the same time, we find that several previously published results need improvement; in particular, we revise the threshold law for $2e^-+e^+$ escape. A general nature of the developed method is illustrated by a consideration of new complicated situations with up to six charged particles in the final state, where a number of threshold exponents is predicted.

In Sec. II we introduce particular configurations which will be called *scaling configurations* (SC's). They describe a multidimensional dynamic potential saddle, generalizing the *Wannier ridge* which is well known for the $2e+$ion system. These configurations are related to *rectilinear trajectories of all particles* in the system, and play a crucial role for the complete fragmentation process close to its threshold. SC's embrace the essence of previous treatments of particular systems, but avoid attachment to some special theoretical formalism and related technical complications. The closest analog to our general approach in the particular case of three-body Coulomb systems can be found in papers by Simonović and Grujić [33].

A description of small deviations from SC's is given in terms of a set of harmonic oscillators and inverted oscillators (Sec. III). The latter describe unstable modes which govern the threshold law. They are quantized following a general scheme suggested by Kazansky and Ostrovsky [34,35]. This allows us to construct a reduced form of the wave function for the system of charged particles, and derive the threshold law in Sec. IV, generalizing a procedure used previously by Kazansky and co-workers [4,12] for a derivation of the conventional Wannier law. Application of a developed general scheme to some particular systems (Sec. V) is followed by a

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concluding discussion of special features of Wannier-type threshold laws, with an emphasis on the relation between the underlying statistical and dynamical aspects of the problem (Sec. VI).

II. SCALING EXPANSION

Our goal is to consider some atomic process which breaks an atomic particle into several charged fragments for low excess energy E. In this situation the motion of the fragments in the final state of the reaction can be described in the semiclassical approximation, because a typical variation of the Coulomb potential $U_C \sim 1/r$ on the wavelengths of the fragments $\lambda \sim 1/\sqrt{ME}$, $\delta U \simeq \lambda/r^2$, is less than a typical kinetic energy $T \sim E$,

$$\delta U \ll T,$$

inside the Coulomb zone $r \gtrsim r_C = 1/E$ where the major events take place. Therefore the first thing to do is to find classical trajectories which lead to the desired final state with total fragmentation.

It is very important that for a low energy E there exists a severe restriction on these trajectories. To see this, let us imagine what is happening with distances separating fragments when they move out of the reaction domain. If a distance separating some pair of attracting fragments diminishes with time, then one should expect that this pair of fragments can be considered as a dipole which interacts with the rest fragments. This interaction can transfer the kinetic energy of the two fragments to the other fragments. Therefore, one has to expect that eventually these two fragments will lose energy and form a bound state. If this event happens, then the desired *total* fragmentation is not achieved. This discussion shows that one should look for those trajectories which exhibit a monotonic increase of distances separating the fragments. The point is that the lower the available above-threshold energy, the more restrictive this condition is.

It is convenient to present this situation by considering the potential energy in multidimensional configuration space, where its behavior can be described as ''valleys separated by ridges.'' This physical picture, first suggested by Wannier for a particular class of reactions, was discussed by Fano [36,37] in a general case. If a system occupies some place on some ridge, then its trajectory can either go down into some valley where a bound state of some fragments is created, or continue to propagate along the ridge. For the total fragmentation, one should find a classical trajectory along the top of some ridge which leads from the region of small separation of fragments into the final state with infinite separation. It is clear that, the lower the above-threshold energy, the closer the trajectory should be to the top of the ridge.

Generally speaking, there might exist several such ridges which lead to the final state with total fragmentation. In this work we study a particular ridge, which will be called the scaling configuration. For all systems considered up to now, we have found that this configuration exists. More than that, for a given system there may exist several different SC's. A number of examples demonstrating this property is considered in Sec. V. Therefore, one might suspect that the SC is a general feature, though this latter statement has not been verified so far. For two electrons in the field of an ion, this ridge coincides with the Wannier ridge.

The basic idea is simple. As stated above, one has to be sure that distances separating fragments increase monotonically with time. This condition is definitely satisfied if a trajectory describing N particles which have masses m_j ($j = 1,2, \ldots, N$) obeys the conditions

$$\vec{r}_j(t) = \phi(t)\vec{\rho}_j, \quad j = 1,2, \ldots, N, \tag{1}$$

which are valid in the center-of-mass reference frame $\Sigma_j m_j \vec{r}_j(t) = 0$. We shall refer to a trajectory satisfying Eq. (1) as a SC. The time-independent vectors $\vec{\rho}_j$ describe the shape of the SC, while the function $\phi(t)$ gives the overall scaling factor. We will see below that this function increases monotonically in time, thus ensuring that all distances increase as well. Therefore, this type of motion definitely results in total fragmentation, avoiding traps into potential valleys. It is convenient to normalize the scaling function to unity for some initial moment of time t_0,

$$\phi(t_0) = 1. \tag{2}$$

For this normalization, the vectors $\vec{\rho}_j$ play a role of coordinates of the particles at this initial moment of time $\vec{r}_j(t_0) = \vec{\rho}_j$ in the center-of-mass reference frame

$$\sum_j m_j \vec{\rho}_j = 0. \tag{3}$$

Notice that in SC's all degrees of freedom except the one describing the overall scaling factor are frozen. In this sense the SC describes a *quasiequilibrium* of the system.

It is obvious that to satisfy Eq. (1) one should appropriately choose the initial coordinates $\vec{\rho}_j$. Let us formulate restrictions on them. Notice, first of all, that in the SC the accelerations of the particles are

$$\frac{d^2\vec{r}_j(t)}{dt^2} = \frac{d^2\phi(t)}{dt^2}\vec{\rho}_j. \tag{4}$$

We presume purely Coulomb interaction, or consider a Coulomb asymptote in more complicated cases, which is possible because the important distances are large ($r \sim r_C = 1/E$) for low above-threshold energy. Therefore the potential energy of the system of N fragments is

$$U = \sum_{m>n} \frac{q_m q_n}{|\vec{r}_m - \vec{r}_n|}. \tag{5}$$

Here q_j is a charge of a jth fragment. The forces $\vec{F}_j$ for a SC are time scaled as

$$\vec{F}_j(t) = -\frac{\partial U}{\partial \vec{r}_j} = \frac{1}{\phi(t)^2}\sum_{n \neq j} q_j q_n \frac{\vec{\rho}_{jn}}{\rho_{jn}^3}, \tag{6}$$

where $\vec{\rho}_{jn} = \vec{\rho}_j - \vec{\rho}_n$. Substituting Eqs. (4) and (6) into the Newton equation of motion, one finds the relation

$$\frac{d^2\phi(t)}{dt^2}m_j\vec{\rho}_j=\frac{1}{\phi(t)^2}\sum_{n\neq j}q_jq_n\frac{\vec{\rho}_{in}}{\rho_{in}^2}. \tag{7}$$

It is easy to see that it can be satisfied only if two conditions are fulfilled. First, the scaling function should satisfy an equation

$$\frac{d^2\phi(t)}{dt^2}=-\frac{\alpha}{\phi(t)^2}, \tag{8}$$

where $\alpha>0$ is a time-independent constant which is discussed in detail below. One obviously recognizes in Eq. (8) the equation describing a one-dimensional motion of a particle with unit mass and unit charge in the attractive Coulomb field created by the charge α. Second, the validity of Eq. (7) requires that the vectors $\vec{\rho}_j$ satisfy the following system of equations:

$$\alpha\vec{\rho}_j=-\vec{a}_j\equiv-\frac{1}{m_j}\sum_{k\neq j}q_jq_k\frac{\vec{\rho}_{jk}}{\rho_{jk}^3}. \tag{9}$$

These equations state that accelerations of each fragment $\vec{a}_j$ are proportional to its coordinate vector at the initial moment of time. Equations (9) are shown to arise as conditions which are necessary for existence of a SC. It is easy to see that they provide sufficient conditions as well. To verify this statement, let us assume that we have a solution of Eq. (9). Then we can consider a trajectory with the following initial conditions. First, we can choose initial coordinates as $\vec{r}_j(t_0)=\vec{\rho}_j$. Second, we can always choose initial velocities that are proportional to coordinates,

$$\frac{d\vec{r}_j(t_0)}{dt}=\beta r_j(t_0), \tag{10}$$

where β is some positive constant which depends on the energy $\beta\sim\sqrt{E}$. From Eq. (9), we find that accelerations at the initial moment of time are also proportional to coordinates,

$$\frac{d^2\vec{r}_j(t_0)}{dt^2}=-\alpha\vec{r}_j(t_0). \tag{11}$$

Thus, for the considered trajectory, both the velocities and accelerations depend linearly on coordinates at the initial moment of time. Combining this fact with the Newton equations of motion, we conclude that the velocities (and accelerations) remain proportional to the coordinates for any moment of time,

$$\frac{d\vec{r}_j(t)}{dt}=\beta(t)\vec{r}_j(t). \tag{12}$$

Here $\beta(t)$ is some positive function $\beta(t_0)=\beta$. Integrating Eq. (12), we conclude that the time variation of distances does exhibit the scaling condition (1), in which $\dot{\phi}(t)=\beta(t)$.

This discussion shows that the SC defined in equation (1) exists if and only if Eqs. (9) are satisfied. There are N vector variables $\vec{\rho}_j$, $j=1,2,\ldots,N$ and one scalar variable α in these equations. Obviously not all of them are independent, because there are seven transformations which do not change the given SC. Three of them correspond to shifts of the SC center of mass. Three others describe rotations of the SC as a whole. One more transformation describes the overall scaling of the SC

$$\vec{\rho}_j\rightarrow\vec{\rho}_j'=\lambda\vec{\rho}_j,\quad j=1,2,\ldots,N, \tag{13}$$

$$\alpha\rightarrow\alpha'=\lambda^{-3}\alpha, \tag{14}$$

with $\lambda>0$. According to Eq. (8), the scaling of α [Eq. (14)] should be accompanied by a corresponding scaling of $\phi(t)$, namely, $\phi(t)\rightarrow\phi'(t)=\lambda^{-1}\phi(t)$. Notice that the latter transformation can be interpreted as a shift of the initial moment of time,

$$t_0\rightarrow t_0', \tag{15}$$

where, according to Eq. (2), t_0' should satisfy

$$\phi'(t_0')=\lambda^{-1}\phi(t_0')=1. \tag{16}$$

It is easy to see that Eqs. (9) remain invariant under the seven transformations discussed above, i.e., the shifts, rotations, and scaling, allowing one to consider them as a set of $3N-7$ equations for $3N-7$ independent variables. When solving these equations it is convenient to treat α as a constant parameter which governs the overall scale, and can be chosen arbitrary (for example, $\alpha=1$).

At the SC, the system Hamiltonian

$$H=\sum_{j=1}^{N}\frac{\vec{p}_j^2}{2m_j}+U,\quad \vec{p}_j=m_j\frac{d\vec{r}_j}{dt} \tag{17}$$

is reduced to

$$H_0=\frac{1}{2}\mathcal{M}\left(\frac{d\phi}{dt}\right)^2-\frac{\mathcal{Q}_0}{\phi}, \tag{18}$$

where

$$\mathcal{M}=\sum_{j=1}^{N}m_j\vec{\rho}_j^2, \tag{19}$$

$$\mathcal{Q}_0=-\sum_{i>j}\frac{q_iq_j}{|\vec{\rho}_i-\vec{\rho}_j|}. \tag{20}$$

Clearly the Hamiltonian (18) describes the one-dimensional motion of a particle with the mass $\mathcal{M}$ and unit charge in the attractive field of a Coulomb center with the charge $-\mathcal{Q}_0$. The corresponding equation of motion is given by Eq. (8), considered previously, in which the constant α proves to be equal to

$$\alpha=\frac{\mathcal{Q}_0}{\mathcal{M}}. \tag{21}$$

The interesting physical events take place if there is sufficient Coulomb attraction in the system. That is why we sup-

pose that the effective Coulomb charge $\mathcal{Q}_0$ is attractive, $\mathcal{Q}_0 > 0$, resulting in a positive value of α.

Equations (19)–(21) show that arbitrary scaling of α can be compensated for by the corresponding scaling of coordinates ρ_j. This fact agrees with Eqs. (13) and (14).

The scaling function $\phi(t)$ is defined by straightforward integration of Eq. (8),

$$\frac{1}{2}\mathcal{M}\left(\frac{d\phi}{dt}\right)^2 - \frac{\mathcal{Q}_0}{\phi} = E, \tag{22}$$

where E is the system energy. Combined with the initial condition $\phi(t_0)=1$, this fixes the scaling function unambiguously.

It is important to emphasize that Eqs. (1) and (9) present the idea of a SC in an invariant form independent of the chosen coordinate frame. To see this more clearly, let us introduce grand vectors in the $3N$-dimensional configuration space. The grand vector $\mathbf{r}(t)=(\vec{r}_1(t), \ldots, \vec{r}_N(t))$ defines the time-dependent coordinates, the vector $\boldsymbol{\rho} = (\vec{\rho}_1, \ldots, \vec{\rho}_N)$ gives the initial coordinates and $\mathbf{a} = (\vec{a}_1, \ldots, \vec{a}_N)$ is the vector of accelerations at the initial moment of time. We employ bold type to distinguish such a vector from the conventional vector in space. Equations (1) and (9) allow the following presentation:

$$\mathbf{r}(t) = \phi(t)\boldsymbol{\rho}, \tag{23}$$

$$\alpha\boldsymbol{\rho} = -\mathbf{a}. \tag{24}$$

Obviously, these relations between $3N$ vectors do not depend on a reference frame. This shows that the scaling coordinate $\phi(t)$ is described in an invariant way.

It has been presumed by previous authors that some coordinate which describes fragmentation is to be singled out, and the potential extremum point is to be found for a fixed value of this ''breakup coordinate.'' The latter has been chosen in most cases as the system hyperradius [36–39] defined as $R^2=\Sigma_{i=1}^{N} m_i r_i^2$. In the hypercoordinate reference frame, the potential energy

$$V = \frac{C(\omega)}{R} \tag{25}$$

is proportional to the hypercharge $C(\omega)$, which depends on a set of hyperangles $\omega=(\omega_1, \ldots, \omega_{3N-7})$. It is easy to verify that definition of the SC equation (24) in the hyperspherical coordinates is reduced to

$$\frac{\partial C(\omega)}{\partial \omega_i} = 0, \tag{26}$$

which shows that the SC is a saddle point of the hypercharge $C(\omega)$. The function $\phi(t)$ in hyperspherical coordinates is proportional to the hyperradius $\phi(t)=R/R_0$, where R_0 is the initial value of the hyperradius. The effective charge $\mathcal{Q}_0$ and the effective mass $\mathcal{M}$ can be expressed in terms of R_0 and the hypercharge $\mathcal{M}=R_0^2$, $\mathcal{Q}_0=-C_0/R_0$, where C_0 is the hypercharge evaluated for SC. A description of the system in hypercoordinates has a long tradition and list of achievements; see, for example, recent calculations of the three-electron atom in hyperspherical coordinates [40]. However, generally speaking, these coordinates do not possess fundamental advantages over other coordinate frames for the fragmentation problem.

Another well-known reference frame provides Jacoby coordinates used in the approach developed by Feagin [41]. For multiparticle fragmentation, the choice of the breakup coordinate is not obvious, and some special procedure was developed for its construction [29,30,19]. This problem becomes more sophisticated the more complicated the system is. In conclusion, it should be stressed once more that our approach provides an invariant definition for the idea of a SC which is given in Eqs. (23) and (24).

III. SMALL DEVIATIONS FROM SCALING CONFIGURATION

Assuming that the function $\phi(t)$ is defined as described in Sec. II, we switch from $\vec{r}_j$ to the new coordinates $\delta\vec{r}_j$,

$$\vec{r}_j = \phi(t)\vec{\rho}_j + \delta\vec{r}_j, \tag{27}$$

which have the obvious meaning of deviations from the SC. Presuming that these deviations are small, we write linearized classical Newtonian equations for $\delta\vec{r}_j(t)$ as

$$m_i\frac{d^2\delta\vec{r}_i}{dt^2} = -\frac{1}{\phi(t)^3}\sum_{j=1}^{N} V_{ij}\delta\vec{r}_j, \tag{28}$$

$$V_{ij} = \frac{\partial^2}{\partial\vec{\rho}_i\partial\vec{\rho}_j}\sum_{m>n}\frac{q_m q_n}{|\vec{\rho}_m-\vec{\rho}_n|}. \tag{29}$$

These equations of motion are generated by the time-dependent Hamiltonian function

$$\delta H = \frac{1}{2}\sum_{j=1}^{N}\frac{\delta\vec{p}_j^{\,2}}{m_j} + \frac{1}{2\phi(t)^3}\sum_{i,j=1}^{N} V_{ij}\delta\vec{r}_i\cdot\delta\vec{r}_j, \qquad \delta\vec{p}_j \equiv m_j\frac{\delta\vec{r}_j}{dt}. \tag{30}$$

It is convenient to introduce scaled deviations $\vec{\xi}_j$ and related momenta $\vec{\pi}_j$ as

$$\vec{\xi}_j = \frac{1}{\phi(t)^{3/4}}\delta\vec{r}_j, \quad \vec{\pi}_j = \phi(t)^{3/4}\delta\vec{p}_j, \tag{31}$$

since this allows us to factor out the time dependence in the Hamiltonian:

$$\delta H = \frac{1}{\phi(t)^{3/2}}\left[\frac{1}{2}\sum_{j=1}^{N}\frac{\vec{\pi}_j^{\,2}}{m_j} + \frac{1}{2}\sum_{ij} V_{ij}\vec{\xi}_i\vec{\xi}_j - \frac{3}{8}\sqrt{\phi}\,\frac{d\phi}{dt}\sum_{j=1}^{N}(\vec{\xi}_j\cdot\vec{\pi}_j + \vec{\pi}_j\cdot\vec{\xi}_j)\right]. \tag{32}$$

The derivation of this formula could be traced via a quantum-mechanical analog of the problem (which for many readers nowadays is more convenient than the pure classical

consideration). In quantum mechanics, the transformation rules for momenta and the Hamiltonian follow, respectively, from the formulas for the partial derivatives:

$$\frac{\partial}{\partial \vec{r}_j} = \phi(t)^{-3/4} \frac{\partial}{\partial \vec{\xi}_j},$$

$$\left(\frac{\partial}{\partial t}\right)_{\delta \vec{r}_j} = \left(\frac{\partial}{\partial t}\right)_{\vec{\xi}_j} + \frac{3}{4\phi(t)^{1/4}} \frac{d\phi}{dt} \sum_{j=1}^{N} \vec{\xi}_j \cdot \frac{\partial}{\partial \delta \vec{r}_j}. \quad (33)$$

In Eq. (32), we use a symmetrized representation which should be employed in the quantum version of the formulas (the latter also implies a corresponding gauge transformation for the wave function).

From Eq. (22), one obtains

$$\sqrt{\phi}\, \frac{d\phi}{dt} = \sqrt{\frac{2[E\phi(t) + \mathcal{Q}_0]}{\mathcal{M}}}, \quad (34)$$

which becomes time independent for $E=0$. In this case the time dependence is *exactly* factored out in the Hamiltonian (32), justifying the choice of the scaling (31). This implies that the original *nonstationary* problem becomes *stationary*, provided one replaces time t by an effective time τ. A relation between t and τ in differential form is

$$d\tau = \phi(t)^{-3/2} dt. \quad (35)$$

For some applications it is necessary to keep the energy dependence of the trajectory. For these cases a convenient technique was developed recently by Kuchiev [17]. We have applied it to the case considered, and verified that it results in the same threshold indexes as the ones obtained below by the stationary approach.

The Hamiltonian describing propagation in the effective time (35) reads

$$\delta H_\tau = \frac{1}{2} \sum_{j=1}^{N} \frac{\vec{\pi}_j^2}{m_j} + \frac{1}{2} \sum_{ij} V_{ij} \vec{\xi}_i \vec{\xi}_j + \frac{a}{2} \sum_{j=1}^{N} (\vec{\xi}_j \cdot \vec{\pi}_j + \vec{\pi}_j \cdot \vec{\xi}_j), \quad (36)$$

$$a = -\frac{3}{4} \sqrt{\phi} \frac{d\phi}{dt}. \quad (37)$$

The Hamiltonian δH_τ [Eq. (36)] is quadratic in coordinates and momenta, thus describing a set of harmonic oscillators or inverted oscillators. This shows that our goal is to describe the behavior of the system in terms of these oscillators and inverted oscillators. Before proceeding, we modify our notation. The set of components of the displacements vectors $\delta \vec{r}_j$ $(j=1,2, \ldots, N)$ comprise a $3N$-dimensional grand vector $\delta \mathbf{r}$. In this formulation, for instance, V_{ij} corresponds to grand $3N \times 3N$ square matrix denoted below as $\mathbf{V}$. We also introduce $3N \times 3N$ unit matrix $\mathbf{I}$ and the diagonal matrix $\mathbf{K}$ of the same size with diagonal elements corresponding to the inverse mass $1/m_j$ of each particle.

This notation takes into account an obvious fact that the total number of all modes coincides with the number of degrees of freedom in the system $(k=1,2, \ldots, 3N)$. There are, however, seven particular degrees of freedom: translations, rotations, and the scaling transformation. They do not change the shape of a SC and do not describe a deviation from a SC. These degrees of freedom may be called the collective modes. They obviously should be considered separately from the oscillating modes which describe deviations from the SC. In order to distinguish the collective modes, one can use the following interesting property. All collective degrees of freedom are described by the eigenvectors of the grand matrix $\mathbf{KV}$ with particular eigenvalues. First, the three modes which correspond to the system translations in space have obviously zero eigenvalues. Second, the modes corresponding to rotations of the system in space have eigenvalues equal to $\mathcal{Q}_0/\mathcal{M}$, as shown in the Appendix. There are three such modes in the general case, while for a linear SC there are only two modes. Third, the mode corresponding to the scaling transformation Eqs. (13) and (14) has an eigenvalue $-2\mathcal{Q}_0/\mathcal{M}$, as also shown in the Appendix. Using these eigenvalues, one can separate the collective modes either from the very beginning, or at the end of calculations.

There is another way, useful for applications, to separate the collective modes. For translations and rotations the separation can be fulfilled by conventional methods choosing appropriately the coordinates, as demonstrated in a number of examples below. Separation of the scaling mode can be achieved with the help of the operator of projection on this mode $\mathbf{P}$ and the complementary projection operator $\mathbf{Q}=\mathbf{I}-\mathbf{P}$. The operator $\mathbf{P}$ is readily constructed from the unit vectors $\vec{n}_j = \vec{\rho}_j/\rho_j$, which define the shape of a SC:

$$P_{ij} = \vec{n}_i \cdot \vec{n}_j. \quad (38)$$

Thus all seven collective modes can be easily identified and separated using any of the two techniques described above.

Some modes in the $3N-7$ subspace orthogonal to the collective modes are stable and describe small oscillations around the SC; the related oscillating frequencies ω_k are real. The object of our major interest is unstable modes with imaginary oscillating frequencies. It is shown below that unstable modes exist for any SC. It is convenient to introduce, for unstable modes, a parameter $\alpha_k = i\omega_k$ $(\mathrm{Re}\ \alpha_k > 0)$. In order to find the oscillating frequencies, one can presume a harmonic time dependence of the coordinates ξ and momenta π,

$$\boldsymbol{\xi} = \exp(i\omega t)\boldsymbol{\Xi}, \quad \boldsymbol{\pi} = \exp(i\omega t)\boldsymbol{\Pi}, \quad (39)$$

where $\boldsymbol{\Xi}$ and $\boldsymbol{\Pi}$ are time-independent grand vectors. The Hamiltonian equations of motion give

$$i\omega\boldsymbol{\Xi} = \mathbf{K}\boldsymbol{\Pi} + a\boldsymbol{\Xi}, \quad i\boldsymbol{\Pi} = -\mathbf{V}\boldsymbol{\Xi} - a\boldsymbol{\Pi}, \quad (40)$$

where a [Eq. (37)] is a scalar coefficient. The latter equation could also be written as

$$i\omega \begin{pmatrix} \boldsymbol{\Xi} \\ \boldsymbol{\Pi} \end{pmatrix} = \begin{pmatrix} a & \mathbf{K} \\ -\mathbf{V} & -a \end{pmatrix} \begin{pmatrix} \boldsymbol{\Xi} \\ \boldsymbol{\Pi} \end{pmatrix}. \quad (41)$$

Excluding the grand vector $\boldsymbol{\Pi}$, one comes to the eigenvalue problem for the square of frequency ω^2,

$$(\omega^2 + a^2)\boldsymbol{\Xi} = \mathbf{KV}\boldsymbol{\Xi}, \quad (42)$$

or, in symmetrized form,

$$(\omega^2+a^2)\tilde{\Xi}=\mathbf{K}^{1/2}\mathbf{V}\mathbf{K}^{1/2}\tilde{\Xi},\quad \mathbf{K}^{1/2}\tilde{\Xi}=\Xi. \tag{43}$$

Denoting a set of eigenvalues of the matrix **KV** as v_k, $k=1,2,\ldots,3N$, we obtain

$$\omega_k^2=v_k-a^2, \tag{44}$$

$$\alpha_k=\sqrt{a^2-v_k}. \tag{45}$$

This formula shows how the oscillation frequencies depend on the eigenvalues of the matrix **KV**.

Let us verify now that a SC is always unstable. With this purpose, let us show that the matrix **KV** always possesses negative eigenvalues which describe instability. Consider the trace of the grand matrix **V**,

$$\mathrm{Tr}\mathbf{V}=\sum_j \frac{\partial^2}{\partial\vec{\rho}_j\partial\vec{\rho}_j}\sum_{m>n}\frac{q_m q_n}{|\vec{\rho}_m-\vec{\rho}_n|}$$

$$=\sum_j \triangle_{\vec{\rho}_j}\sum_{m>n}\frac{q_m q_n}{|\vec{\rho}_m-\vec{\rho}_n|}=0, \tag{46}$$

which vanishes since the Coulomb potential satisfies the Laplace equation

$$\Delta_{\vec{\rho}_j}\frac{1}{|\vec{\rho}_j-\vec{\rho}_n|}=0,\quad \vec{\rho}_j\neq\vec{\rho}_n.$$

It is easy to see also that Eq. (46) results in $\mathrm{Tr}(\mathbf{KV})=0$ which means that

$$\mathrm{Tr}(\mathbf{KV})=\sum_k v_k=0. \tag{47}$$

We see that the spectrum of the matrix **KV** always contains both positive and negative eigenvalues. This fact in itself is not sufficient to make a statement about instability, because trace (47) includes a contribution from collective modes which do not change the shape of the SC. However, it is easy to exclude collective modes. Remember that the eigenvalues corresponding to translations are zero, and rotations give eigenvalues $\mathcal{Q}/\mathcal{M}$, while the scaling transformation provides the eigenvalue $-2\mathcal{Q}/\mathcal{M}$; see the Appendix. The sum of eigenvalues of collective modes is

$$\sum_{\text{collective modes}} v_k=\begin{cases}\mathcal{Q}/\mathcal{M} & \text{in the general case}\\ 0 & \text{for a linear SC.}\end{cases} \tag{48}$$

Subtracting this result from Eq. (47), we find the trace of the matrix **KV** in the subspace orthogonal to the collective modes,

$$\mathrm{Tr}(\mathbf{K}\,\mathbf{V})_{\text{orth}}=\sum_{\text{orthogonal}} v_k=\begin{cases}-\mathcal{Q}/\mathcal{M} & \text{in the general case}\\ 0 & \text{for a linear SC.}\end{cases} \tag{49}$$

Since this trace is nonpositive, we conclude that the matrix **KV** inevitably possesses negative eigenvalues which describe deviations from the SC. This shows that any SC is unstable. This property is closely related to the fact that harmonic functions, i.e., those which satisfy the Laplace equation, cannot have maxima or minima. Remember also the Earnshow theorem, well known in electrostatics: stable equilibrium is impossible for systems where the Coulomb forces are operative. Although SC's describe expanding nonstatic configurations, the conclusion about inevitable instability remains valid in this case as well. This fact can be interpreted as a dynamic analogue of the Earnshow theorem.

IV. QUANTIZATION OF DEVIATIONS FROM SCALING CONFIGURATION AND THRESHOLD INDICES

Section III reduces description of small deviations from SC to the set of coupled harmonic oscillators which could be quantized straightforwardly. This procedure provides the ''energy'' levels

$$\epsilon_{kn_k}=\omega_k(n_k+\tfrac{1}{2}). \tag{50}$$

Here the first subscript $k=1,2,\ldots,3N-7$ indicates the mode, and $n_k=0,1,\ldots$ shows a number of quanta in this mode. For a given set of the quantum numbers $\{n_k\}$ the system wave function is given by

$$\Psi_{\{n_k\}}\sim\exp\left(-\sum_k i\int_{\tau_0}^{\tau}\epsilon_{kn_k}d\tau\right)$$

$$=\exp\left(-\sum_k i\int_{t_0}^{t}\frac{\epsilon_{kn_k}}{\phi(t)^{3/2}}dt\right), \tag{51}$$

where we omit the common time-dependent phase factor. The wave function is prepared at some initial moment t_0 by preceding strong interaction of all fragments. In the Wannier-type approach it is presumed that these processes depend smoothly on the energy E. Hence they do not influence the form of the threshold law, and thus could be effectively excluded from consideration; it is sufficient to consider only the $t>t_0$ domain.

For unstable modes the ''energies'' ϵ_{kn_k} are complex valued which leads to the loss of probability in the expanding SC. This should be interpreted [34,35] as a sliding from the potential saddle in multidimensional configuration space that eventually leads to formation of bound states of two (or more) fragments. Such an outcome implies that the related part of the probability is lost for the process of complete system fragmentation which is an object of our study. The cross section of the latter is proportional to the *survival probability*

$$P_{\{n_k\}}\equiv|\Psi_{\{n_k\}}|_{t\to\infty}|^2$$

$$=\exp\left[-\sqrt{2\mathcal{M}}\right.$$

$$\left.\times\sum_k\int_{\phi(t_0)}^{\infty}\frac{\alpha_{kn_k}}{\phi\sqrt{E\phi+\mathcal{Q}_0}}d\phi\left(n_k+\frac{1}{2}\right)\right], \tag{52}$$

where summation over k runs over all unstable modes. Note that the original quantum problem is stationary. The time t in Eq. (52) plays the role of an effective variable which describes the scaling of the system in accordance with Eq. (22).

Small deviations from the SC are described quantum mechanically. Our treatment generalizes to a multimode case the scheme developed by Kazansky and Ostrovsky [4] for the two-electron escape (see also Ref. [12]; some ideas used were also elaborated by Watanabe [2]). Note that the cited paper [4] also provides a description of deviations from a pure power threshold law, but we do not pursue this point here.

For our objectives it is sufficient to note that Eq. (52) has the form of a product of contributions coming from each individual mode; hence the threshold law of interest is

$$\sigma \sim P_{\{n_k\}} \sim E^{\mu}, \tag{53}$$

$$\mu \equiv \sum_k \mu_{kn_k}. \tag{54}$$

The *partial threshold indices* μ_{kn_k} stem from ''eigenfrequencies'' of unstable modes, being related to the *negative* eigenvalues $v_k<0$ of the **KV** matrix,

$$\mu_{kn_k}=2\left[\sqrt{-\frac{\mathcal{M}}{2\mathcal{Q}_0}v_k+\frac{9}{16}}-\frac{1}{4}\right]\left(n_k+\frac{1}{2}\right). \tag{55}$$

Small positive values of v_k could formally also lead to a real μ_{kn_k}, but have to be discarded. Obviously, if some (imaginary) eigenfrequencies are N_k-fold degenerate, the related contributions appear N_k times in the (54). In principle, the wave function is a superposition of terms corresponding to various sets of quantum numbers $\{n_k\}$, since all of them are populated by processes in the inner interaction domain. Clearly, the threshold law is defined by the least possible values of n_k [42], which are equal to zero unless the symmetry considerations forbid this choice, as exemplified in the next paragraph. If the initial SC is scaled by the factor λ [see Eqs. (13) and (14)], then $\mathbf{KV}\sim\lambda^{-3}$, $\mathcal{M}\sim\lambda^2$, and $\mathcal{Q}_0 \sim\lambda^{-1}$, but the threshold indices μ_{kn_k}, as anticipated, remain scale-independent. Note also that the threshold index is invariant under simultaneous scaling of all charges or all masses in the system.

In the original Wannier problem two electrons escape from infinitely heavy atomic core with the charge Z. The configuration found by Wannier [1] gives the simplest example of a SC in which the electrons reside at equal distances ρ and in opposite directions from the core. The motion is unstable with respect to the stretching mode, which is separated from the (stable) bending mode. Thus it is sufficient for our purposes to consider the motion of electrons along the line passing through the core. This motion is described by two coordinates and the matrix **V** takes the form

$$\mathbf{V}=\frac{1}{\rho^3}\begin{pmatrix} -2Z+\frac{1}{4} & -\frac{1}{4} \\ -\frac{1}{4} & -2Z+\frac{1}{4} \end{pmatrix},$$

and $\mathcal{Q}_0=(2Z-\frac{1}{2})\rho^{-1}$ and $\mathcal{M}=2\rho^2$ (we use an atomic system of units, **K=I**). The eigenvalues of **V** are $v_1 =-2Z/\rho^3$ and $v_2=(-2Z+\frac{1}{2})/\rho^3$. The eigenvalue v_2 is seen to coincide with $-2\mathcal{Q}/\mathcal{M}$. Hence it corresponds to SC expansion (see the Appendix) and should be discarded. The eigenvalue v_1, upon substitution into Eq. (55), reproduces the well-known result

$$\mu_{1n_1}=\frac{1}{2}\left[\sqrt{\frac{100Z-9}{4Z-1}}-1\right]\left(n_1+\frac{1}{2}\right). \tag{56}$$

The choice $n_1=0$ provides the famous Wannier law valid for ^1S symmetry of the final two-electron continuum state, whereas $n_1=1$ corresponds to the threshold law for $^3S^e$ (and $^3P^e$) symmetry [43].

Feagin and Filipczyk [29] and Poelstra, Feagin, and Klar [30] put forward another formula for the threshold index in the multimode case. According to this, the Wannier index is $N-2$ times larger than Eq. (54). The factor $N-2$ is described as a ''phase-space factor for $N-1$ outgoing particles'' being justified by the reference to the earlier paper by Feagin [41]. We were unable to find the derivation of such a factor in the cited paper; in any case, it deals only with the conventional $N=3$ case where the factor $N-2$ is insignificant. Our treatment provides a purely dynamic approximation for the wave function, and does not leave any room for the statistical arguments. The other aspects of relation between dynamic and statistical threshold laws are discussed in Sec. VI.

V. PARTICULAR SYSTEMS

In practical applications of our scheme, the less obvious part corresponds to finding SC's. Numerical solution of the set of nonlinear equations (9) could be cumbersome, and implies a reasonable initial guess. The question of whether all the solutions are found is even more difficult. In reality, one has to appeal to intuitive reasoning, and to limit the search to some symmetrical configuration. This allows one to reduce effectively the number of equations (9) to be considered. Since the initial step of finding SC's in most cases could not be done in closed form, we do not pursue the goal of obtaining analytical formulas, but resort to numerical calculations which are performed using the MATHEMATICA [44] program. We find it easier to avoid preliminary separation of rotational and translational coordinates, since they could be easily distinguished in the eigensystem of the complete matrix **KV**. Moreover, the known eigenvalues of this matrix corresponding to rotations (see the Appendix) provide a good test for consistency of calculations.

The systems practically accessible nowadays in atomic physics are not very diverse, consisting of several electrons and positrons in the field of heavy (positively charged) atomic core. Since three-particle systems (such as $A^{+Z}+2e^-$ or $A^{+Z}+e^-+e^+$) have already been studied in great detail [1,38,39,45–47,33] (see also references in Sec. I), we start from four-particle systems. We do not impose any symmetry constraints on the system state, thus presuming that $n_k=0$ for all modes contributing μ [Eq. (54)].

A. Three-electron escape from the charged core

The system $A^{+Z}+3e$ was thoroughly investigated by Klar and Schlecht [22] and Grujić [24]. They considered a configuration of electrons forming an equilateral triangle with an infinitely massive core in the center, which is obvi-

ously a SC. The out-of-plane motion is separated. It corresponds to stable modes, and does not affect the threshold law. The in-plane motion is described by six coordinates of electrons, or by four ''oscillatory'' modes plus a uniform expansion of the SC and its rotation. The eigenfrequencies obtained by us, as well as in the cited papers, are pairwise degenerate due to SC symmetry. One pair corresponds to stable motion, and the other pair to unstable motion. The latter pair produces two equal terms in sum (54). Klar and Schlecht [22] and Grujić [24] succeeded in deriving analytical expressions for the Wannier index [48]. In this paper we do not pursue analytical formulations but check that our numerical results coincide with those cited by Grujić, namely, $\mu=2.826\,24$ for $Z=1$, $\mu=2.270\,43$ for $Z=2$, $\mu=2.161\,96$ for $Z=3$, etc. The experiment for electron-impact double ionization of atoms ($Z=3$) seems to agree with the threshold law [28].

The two pairs of modes discussed above are already well known. Combined with rotation and scaling expansion, they represent a complete set of six in-plane coordinates. Since the number of modes is a physical parameter which is independent of the theoretical technique used, we do not see any possibility to obtain additional unstable modes which would lead to another Wannier index and thus to the complementary threshold law as announced by Feagin and Filipczyk [29] (in fact our conclusion could be drawn from the paper by Grujić [24], who used plain Cartesian coordinates, whereas the less transparent treatment by Klar and Schlecht [22] is based on hyperspherical coordinates). Since no details of the analysis by Feagin and Filipczyk [29] were ever published, a more detailed discussion of this issue is not possible.

B. $2e^-+e^+$ escape from the charged core

The plausible symmetric SC's for the system $A^{+Z}+2e^-+e^+$ were considered in Ref. [30] (note that the calculations in this paper were carried out only for $Z=1$). The authors comprised two different linear arrangements and one plain configuration [49]. All these configurations belong to the SC, and, therefore, can be easily handled by the technique developed above. We consider below these SC's successively.

1. Linear configuration L_a

The linear SC L_a is shown in Fig. 1. The frame origin is placed into an infinitely massive core having the charge Z. The coordinates of two electrons and a positron are x_1, x_2, and x_3, respectively; all of them are positive. It is convenient to introduce two dimensionless parameters $x=r_1/r_3$ and $y=r_2/r_3$ $(0<x<1<y)$, which have to satisfy the system of equations obtained from Eq. (9):

$$\frac{m_3}{m_1}\frac{Z/x^2-1/(1-x)^2+1/(y-x)^2}{-Z+1/(1-x)^2-1/(1-y)^2}=x,$$
$$\frac{m_3}{m_2}\frac{Z/y^2+1/(1-y)^2-1/(y-x)^2}{-Z+1/(1-x)^2-1/(1-y)^2}=y \tag{57}$$

(equations are presented for more general case when all light particles have different masses m_i, while the core remains infinitely heavy).

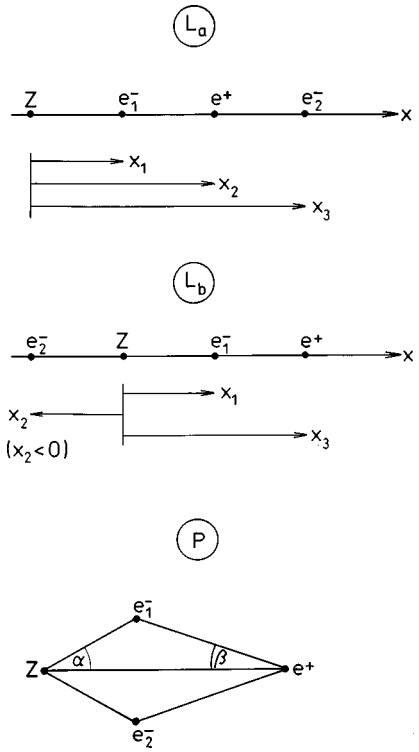

FIG. 1. Two linear and plain scaling configurations for the system $A^{+Z}+2e^-+e^+$.

2. Linear configuration L_b

A distinction from the previous case is that the coordinate of one of the electrons is negative ($x_2<0$). The system of equations defining the SC is somewhat different ($y<0<x<1$):

$$\frac{m_3}{m_1}\frac{Z/x^2-1/(1-x)^2-1/(y-x)^2}{-Z+1/(1-x)^2+1/(1-y)^2}=x,$$
$$\frac{m_3}{m_2}\frac{-Z/y^2-1/(1-y)^2+1/(y-x)^2}{-Z+1/(1-x)^2+1/(1-y)^2}=y. \tag{58}$$

For both linear configurations, the bending modes are stable. There are two stretching modes for each configuration, both unstable. The results of our calculations are summarized in Table I. For $Z=1$ parameters x and y and partial threshold indices μ_1 and μ_2 coincide with those obtained in Ref. [30]; our threshold indices μ are less by a factor of 2, as discussed at the end of Sec. IV. Notice a nontrivial behavior of the parameters with Z: for instance, in the SC L_a, x and μ_1 increase with Z, whereas y and μ_2 decrease. The threshold index μ increases with Z, which is opposite to the well-known behavior for the simplest system A^Z+2e, and for $3e$ escape where μ diminishes as Z grows (see more discussion in Sec. VI).

3. Plane configuration P

The symmetric plane configuration shown in Fig. 1 is conveniently characterized by two angles α and β. From Eq. (9), we deduce the system of equations

TABLE I. Parameters of scaling configurations and Wannier indices for the $A^{+Z}+2e^-+e^+$ system.

Z	SC parameters		μ_1	μ_2	μ
		SC L_a			
1	$x=0.506\,100$,	$y=1.692\,952$	4.442 178	2.193 945	6.636 123
2	$x=0.587\,468$,	$y=1.636\,629$	4.767 141	2.064 237	6.831 377
3	$x=0.633\,155$,	$y=1.609\,587$	5.024 502	1.966 884	6.991 386
4	$x=0.664\,214$,	$y=1.594\,313$	5.242 328	1.88 483	7.127 158
		SC L_b			
1	$x=0.441\,380$,	$y=-0.677\,611$	2.577 720	1.025 435	3.603 155
2	$x=0.539\,724$,	$y=-0.847\,969$	2.888 492	1.009 213	3.897 705
3	$x=0.594\,480$,	$y=-0.949\,091$	3.193 559	1.005 040	4.198 599
4	$x=0.631\,720$,	$y=-1.023\,071$	3.475 766	1.003 244	4.479 010
		SC P			
1	$2\alpha=76.7338°$,	$2\beta=55.1969°$	1.884 950	1.562 234	3.447 184
2	$2\alpha=55.1741°$,	$2\beta=61.3793°$	2.045 028	1.793 101	3.838 128
3	$2\alpha=45.4233°$,	$2\beta=64.1787°$	2.206 553	1.972 092	4.178 645
4	$2\alpha=39.5138°$,	$2\beta=65.8916°$	2.351 217	2.123 469	4.474 686

$$m_+ \sin^3\gamma(Z\sin^2\alpha-\tfrac{1}{4}\sin\alpha+\sin^2\beta\cos\gamma) = m_-\sin^3\beta(2\cos\beta\sin^2\gamma-Z\sin^2\alpha), \qquad (59)$$

$$\sin^2\beta\sin\gamma=\tfrac{1}{4}\cos\alpha \quad (\gamma=\pi-\alpha-\beta),$$

where the masses of light particles with negative (m_-) and positive (m_+) charges generally could be different. The results of calculations are presented in Table I. For $Z=1$, the angles α and β coincide with those extracted from Ref. [30]. However, the difference between the threshold indices is drastic. Poelstra, Feagin, and Klar had found a single unstable mode which corresponds to our partial Wannier index μ_2. Our calculations give two unstable modes, similar to the case of $3e$ escape (in the latter case the modes were degenerate due to a symmetry which is absent for the system under consideration). The reason for this disagreement remains unclear. The plane SC P governs the threshold behavior, although it provides a threshold index μ only slightly less than the linear configuration L_b.

C. Four-electron escape from the charged core

Basing on symmetry considerations, we analyze three configurations: linear, plane, and three-dimensional SC's. It could be shown rigorously that for a symmetric linear arrangement, a SC does not exist for all values of Z, i.e., Eqs. (9) have no solution.

1. Plane configuration P

In the plane configuration the electrons are located in the apexes of a square; the core lies in its center. The out-of-plane motion is separated, and corresponds to stable modes. For in-plane motion in the general case, we find nondegenerate and doubly degenerate unstable modes (Table II). For the particular case $Z=1$, an additional nondegenerate mode becomes unstable.

2. 3D configuration V

The SC describes electrons located at the apexes of tetrahedron. We find a single triply degenerate mode (Table II). Interestingly, the threshold index μ proves to be quite close for plane and three-dimensional (3D) configurations, although the 3D SC provides a somewhat lower value of μ and thus governs the threshold behavior. As Z increases, the relative importance of electron-electron interaction decreases, and μ approaches the value $\mu=3$ which corresponds to noninteracting electrons.

The smallest practically attainable value of the charge seems to be $Z=2$. It could be realized via triple ionization of negative ion by electron impact. However, theoretically the case $Z=1$ proves be very interesting due to unusual properties. In this case the threshold index becomes much larger than in other cases, particularly for the plane SC. This is due to a small value of the ''charge'' $\mathcal{Q}_0$ in this case. Another interesting feature is the appearance of an additional unstable mode in the plane SC. An analysis of the eigenvector Ξ

TABLE II. Wannier indices for $A^{+Z}+4e$ system. The numbers in parentheses indicate the degree of unstable mode degeneracy.

Z	μ_1	μ_2	μ_3	μ
		SC P		
1	4.877 419	4.248 225 (2)	2.071 837	15.445 71
2	1.356 093	1.273 381 (2)	—	3.902 855
3	1.192 808	1.145 660 (2)	—	3.484 128
4	1.132 414	1.099 316 (2)	—	3.331 046
5	1.100 871 (2)	1.075 346	—	3.251 563
		SC V		
1	3.075 960 (3)	—	—	9.227 870
2	1.257 986 (3)	—	—	3.773 958
3	1.139 795 (3)	—	—	3.419 384
4	1.095 940 (3)	—	—	3.287 819
5	1.073 040 (3)	—	—	3.219 120

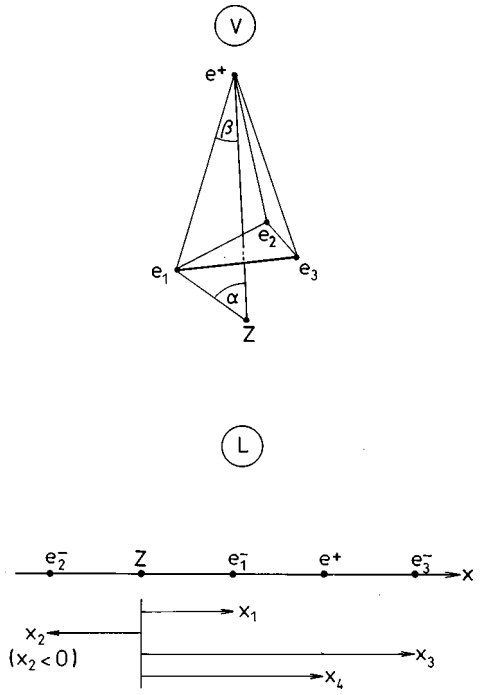

FIG. 2. Linear and 3D scaling configuration for the system $A^{+Z}+3e^-+e^+$.

shows that it corresponds to the out-of-plane motion. That is, a pair of electrons lying on a diagonal of the square shifts upwards, whereas another pair shifts downwards.

The tetrahedric configuration was considered earlier by Grujić [26], who obtained approximate analytical expressions for the threshold indexes. The partial threshold indexes obtained by him reveals only an approximate degeneracy. The numerical results for μ are in reasonable agreement with our data.

D. $3e^-+e^+$ escape from the charged core

We failed to find a symmetrical plane SC for this system.

1. Linear configuration L

A linear SC (Fig. 2) corresponds to alternating positive and negative charges and could be characterized by three parameters: $x=x_1/x_4$, $y=x_2/x_4$, $z=x_3/x_4$ $(y<0<x<1<z)$. They have to satisfy a set of equations which follow from Eq. (9):

$$
\begin{aligned}
&-\frac{Z}{x^2}+\frac{1}{(x-y)^2}+\frac{1}{(1-x)^2}-\frac{1}{(z-x)^2}\\
&\qquad=x\left[Z-\frac{1}{(1-x)^2}+\frac{1}{(z-1)^2}-\frac{1}{(1-y)^2}\right],\\
&\frac{Z}{y^2}-\frac{1}{(x-y)^2}+\frac{1}{(1-y)^2}-\frac{1}{(z-y)^2}\\
&\qquad=y\left[Z-\frac{1}{(1-x)^2}+\frac{1}{(z-1)^2}-\frac{1}{(1-y)^2}\right],\\
&-\frac{Z}{z^2}+\frac{1}{(z-x)^2}+\frac{1}{(z-y)^2}-\frac{1}{(z-1)^2}\\
&\qquad=z\left[Z-\frac{1}{(1-x)^2}+\frac{1}{(z-1)^2}-\frac{1}{(1-y)^2}\right].
\end{aligned}
\tag{60}
$$

The parameters of the SC and the Wannier indices are shown in Table III.

2. 3D configuration V

The symmetrical 3D configuration is shown in Fig. 2. It is characterized by two angles α and β defined by equations similar to Eq. (59):

$$
\begin{aligned}
&m_+\sin^3\gamma\left(Z\sin^2\alpha-\frac{1}{\sqrt{3}}\sin\alpha+\sin^2\beta\cos\gamma\right)\\
&\qquad=m_-\sin^3\beta(3\cos\beta\sin^2\gamma-Z\sin^2\alpha),\\
&\sin^2\beta\sin\gamma=\frac{1}{\sqrt{3}}\cos\alpha\quad(\gamma=\pi-\alpha-\beta).
\end{aligned}
\tag{61}
$$

We found two doubly degenerate unstable modes and one nondegenerate unstable mode, as shown in Table III. The

TABLE III. Parameters of SC's and Wannier indices for $A^{+Z}+3e^-+e^+$ system. The numbers in parentheses indicate the degree of unstable mode degeneracy.

Z	SC parameters	μ_1	μ_2	μ_3	μ
	SC *L*				
1	$x=0.580\,448,\ y=-1.070\,391\ z=1.627\,861$	4.412 13	2.309 76	1.068 90	7.790 79
2	$x=0.580\,448,\ y=-1.070\,391\ z=1.627\,861$	4.738 44	2.132 21	1.033 43	7.904 08
3	$x=0.628\,772,\ y=-1.162\,883\ z=1.602\,043$	4.999 54	2.017 66	1.022 70	8.039 98
4	$x=0.661\,096,\ y=-1.224\,38\ z=1.587\,485$	5.219 72	1.925 98	1.017 46	8.163 16
	SC *V*				
1	$\alpha=60.5698°,\ \beta=32.2041°$	1.575 84 (2)	1.031 94	0.604 93 (2)	5.393 48
2	$\alpha=40.5400°,\ \beta=41.7154°$	1.563 54 (2)	1.200 43	0.663 02 (2)	5.653 56
3	$\alpha=32.3675°,\ \beta=44.9869°$	1.709 57 (2)	1.337 11	0.627 71 (2)	6.011 66
4	$\alpha=27.6668°,\ \beta=46.7663°$	1.851 29 (2)	1.450 98	0.573 27 (2)	6.300 11

TABLE IV. Parameters of SC's and Wannier indices for the $A^{+Z}+5e$ system. The numbers in parentheses indicate degree of unstable mode degeneracy.

Z	SC parameters	μ_1	μ_2	μ_3	μ
		SC P			
2	—	1.818 250 (2)	1.575 289 (2)	0.701 595 (2)	6.787 079
3	—	1.363 938 (2)	1.245 279 (2)	—	5.218 433
4	—	1.235 701 (2)	1.156 156 (2)	—	4.783 715
5	—	1.174 520 (2)	1.114 540 (2)	—	4.578 120
6	—	1.138 614 (2)	1.090 432 (2)	—	4.458 093
7	—	1.114 982 (2)	1.074 705 (2)	—	4.379 373
		SC V			
2	$\alpha=45.15762°$	1.606 923	1.504 688	1.493 106 (2)	6.097 823
3	$\alpha=45.09672°$	1.280 163	1.228 075	1.223 717 (2)	4.955 672
4	$\alpha=45.06976°$	1.182 908	1.147 576	1.145 087 (2)	4.620 659
5	$\alpha=45.05455°$	1.135 887	1.109 091	1.107 406 (2)	4.459 790
6	$\alpha=45.04479°$	1.108 127	1.086 528	1.085 274 (2)	4.365 202
7	$\alpha=45.03799°$	1.089 794	1.071 698	1.070 708 (2)	4.302 909

threshold law is governed by the 3D SC V. Note that the threshold index grows with Z.

E. Five-electron escape from the charged core

1. Plane configuration P

In the plane SC, the electrons are located in the apexes of an equilateral pentagon; the core lies in the same plane. In the in-plane motion we have found two doubly degenerate unstable modes (Table IV). For $Z=2$, an additional pair of unstable modes appears.

2. 3D configuration V

Here three electrons lie in the apexes of an equilateral triangle with the core in its center. Perpendicular to this plane, above the plane and below it, another pair of electrons is located symmetrically (Fig. 3). The SC can be characterized by the angle α between the line which joins the out-of-plane electron with the core and the line which joins it with the in-plane electron. The angle is defined by the equation

$$\frac{1}{\sqrt{3}}+2\sin^3\alpha-Z = \tan\alpha\left(3\sin^2\alpha\cos\alpha+\frac{1}{4}\tan^2\alpha-Z\tan^2\alpha\right). \quad (62)$$

Quite unexpectedly, α proves to be very close to 45°, exhibiting a weak dependence on the core charge Z (Table IV). This means that in-plane and out-of-plane electrons are located at almost the same distance from the core. The 3D SC generates somewhat lower values of μ than the plane SC, thus governing the threshold behavior. However, the difference is quite small. This feature is common to that found above for the four-electron case.

The 3D configuration for five-electron system was considered previously in Ref. [27]. However, the equation derived for the SC angle α differs from Eq. (62).

F. Fragmentation in two pairs of identical particles with opposite charges

In this subsection we consider fragmentation into the final state $2X_m^{+Z}+2e$, where X_m^{+Z} is a positively charged particle with charge Z and mass m (all results below hold if the electrons are replaced by any other charged particles; then Z and m have the meaning of a ratio of charges and masses, respectively). In the applications considered above, the zero eigenvalues of the matrix **V** do not emerge due to the presence of infinitely massive core. In the $2X_m^{+Z}+2e$ system, such modes are present. Another distinction is that for equal masses of leptons in previous applications, we always had $\mathbf{K}=\mathbf{I}$, and v_k were the eigenvalues of the **V** matrix. Now we have to diagonalize the complete matrix **KV**. Neither of these features create substantial difficulties.

From symmetry considerations, it is clear that the shape of the SC is a rhombus, with an angle 2α at the apexes where the particles X_m^Z are situated (Fig. 4). The single SC parameter α is defined by the equation

$$8Z-\frac{Z}{\cos^3\alpha}=m\left(8Z-\frac{1}{\sin^3\alpha}\right), \quad (63)$$

which follows from (9). Several examples are shown in Table V. The simplest practical realization is the complete fragmentation of the H_2 molecule by photons, where α is close to 30° in agreement with Feagin and Filipczyk [29], and the threshold index proves to be huge. Apparently this threshold behavior could not be observed in experiments [50]. Another feasible realization with a moderate Wannier index is ionization of a negative positronium ion by positron impact ($Z=1$, $m=1$). We fail to find the linear configuration discussed by Stevens and Feagin [31].

VI. DISCUSSION AND CONCLUSION

This paper formulates the idea of the SC. Defined by Eq. (1), the SC is shown to arise when a nonlinear set of Eqs. (9) is satisfied. Propagation of the system in the vicinity of the

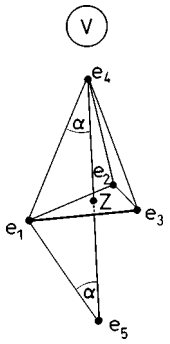

FIG. 3. 3D scaling configuration for the system $A^{+Z}+5e^{-}$.

SC configuration governs the threshold law which is found in Eqs. (53), (54), and (55). These results permit direct practical calculations of the threshold index μ for any system.

In many cases, the threshold laws in quantum mechanics can be deduced from general considerations without dynamical treatment. For instance, the breakup cross section with N fragments in the final state and a short-range interaction between them could be estimated from simple phase-space volume (i.e., statistical) arguments as

$$\sigma_{\mathrm{S}} \sim E^{(3/2)(N-1)-1}. \tag{64}$$

If one presumes that all fragments (''electrons'') are *attracted* by Coulomb forces to one fragment (''core''), but the interaction between the ''electrons'' is negligible, then the phase-space arguments could be easily modified to give

$$\sigma_{\mathrm{C}} \sim E^{N-2}. \tag{65}$$

In the case of a *repulsive* Coulomb interaction with the ''core'' (but still without other interfragment interactions), the cross section at the threshold becomes exponentially small, as obtained, for example, by Geltman [51] in his calculations for atom ionization by positron impact with all correlation neglected. The threshold behavior changes to $\sim E^{3/2}$ [52] if one employs the so-called $3C$ wave functions for the final continuum state. However, these functions do not ensure a proper description in the near-threshold domain.

If one aims to obtain a correct threshold law for the Coulomb system, then the interaction between the fragments, i.e., *the particle correlation*, is to be taken into account. This makes the phase-space arguments insufficient, but requires a dynamical treatment, as was originally done by Wannier [1] for the simplest system. In this paper we employ the most simple theoretical apparatus, presenting essential equations in an arbitrary coordinate frame. They remain valid, in particular, in the simplest single-particle Cartesian coordinates.

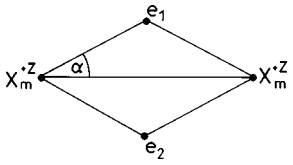

FIG. 4. Plane scaling configuration for the system $2X_m^{Z}+2e^{-}$.

As discussed in Sec. IV, Poelstra, Feagin, and Klar [30] suggested another formula for the Wannier index which differs from our Eq. (54) by the extra ''phase factor'' $N-2$. This discrepancy remains hidden when one restricts consideration to the case of two, three, or four electrons receding from the positively charged core. In these cases the unstable mode proves to be, respectively, nondegenerate, doubly degenerate, and triply degenerate. Thus the degree of degeneracy *in these cases* coincides with $N-2$. This fortuitously allows one to replace the summation over degenerate modes implied by formula (54) by multiplication over the factor $N-2$, which corresponds to the formula in Ref. [30]. However, this coincidence is accidental and misleading. It is broken, for instance, by variation of charges and masses of the constituent particles which violates the SC's symmetry, and hence lifts the mode's degeneracy, or by considering larger numbers of particles N (simply because possible degrees of degeneracy are restricted by properties of the point groups in 3D space). For five electrons receding from a charged core, only doubly degenerate unstable modes were found above.

Physically it is clear that if the charge of the core Z in the system $A^{Z}+(N-1)e$ becomes larger, then the interelectron correlations should become less important and the threshold law should approach the value obtained from the phase-space arguments, i.e., $\mu \to (N-2)$ as $Z \to \infty$. This conclusion is supported by all examples considered. Moreover in all these examples one can note that: (i) the number of unstable modes accounting for their degeneracy [i.e., the number of terms in sum (54)] is equal to $N-2$, and (ii) each partial Wannier index μ_{k0} [Eq. (55)] tends to unity from above as Z increases.

An apparent exception from rule (i) is an emergence of an additional unstable mode in the plane $A^{+Z}+4e$ SC for $Z=1$. However, this SC provides μ larger than the 3D SC, and therefore it does not govern the threshold behavior. Note that although these properties are physically very natural, it is not clear if they can be proven rigorously from first principles. An additional observation is that the electrons in the SC tend to be distributed uniformly on the sphere, even when the corresponding perfectly symmetrical body does not exist (see the five-electron case above). For a large number of electrons in the field of the core, several competing SC's are found to produce very close threshold indices. Still, in all the cases

TABLE V. Parameters of SC's and Wannier indices for the $2X_m^{Z}+2e$ system. The numbers in parentheses indicate the degree of unstable mode degeneracy.

Z	m	α	μ_1	μ_2	μ_3	μ
1	1	$\alpha=45°$	1.293 66	0.905 84 (2)	—	3.105 33
2	1	$\alpha=32.2093°$	1.367 62	1.336 43	—	2.704 05
1	2	$\alpha=35.9490°$	1.569 58	1.317 88	0.543 15	3.430 62
1	1836	$\alpha=30.0049°$	50.329 79	37.462 32	—	87.792 11

considered, the leading SC is found to be the three-dimensional one.

These results hopefully should hold if the electrons are replaced by other (possibly different) negatively charged particles. However, the situation changes drastically if one of the ''electrons'' is replaced by a particle of positive charge, for example, a positron. It is essential that an additional *repulsive Coulomb interaction* appears in the system. If correlations are neglected, then the cross section decreases exponentially as E approaches threshold. One could expect that although the true threshold law retains a power character for all values of Z, it tends to mock the exponential behavior by increasing the value of μ [53]. This property holds for all positron-containing systems considered above. The threshold index increases quite slowly with Z. In order to illustrate the later point quantitatively, we cite results for the $A^{+Z}+2e^{-}+e^{+}$ system with very large values of Z (cf. Sec. V B): $\mu=9.4$ for $Z=50$ ($\alpha=5.60°$, $\beta=37.2°$), and $\mu=11.6$ for $Z=100$ ($\alpha=3.95°$, $\beta=37.8°$). In general terms, one can argue that a similar situation should arise when a system contains two or more positively charged particles *and* two or more particles with negative charge. Note that the properties of the partial Wannier indices μ_{k0} are less straightforward: some of them could be less than unity, and vary with Z nonmonotonically.

Large values of threshold indexes μ are unfavorable for an experimental observation of the threshold behavior: close to the threshold the cross section proves to be too small to be observable, and for higher excess energies the intrinsic deviations from the threshold law become essential. An analysis of the energy domain where the threshold law holds is beyond the scope of this paper. Still, we can note that for the electron-impact ionization of atoms or for double photoionization this domain is limited to few eV above threshold (for a quantitative treatment within the Wannier mechanism, see Refs. [4,12]). For the positron-impact ionization the applicability domain is even less [12,13]. As argued by Ihra *et al.* [18], an agreement with experimental data could be substantially improved if the interaction of different modes in the deviation from SC's is taken into account. Possibly some procedure to assess for the mode interaction could also be developed for the multifragment system; the present development provides a necessary first step for more advanced approaches. One could also note that even very large threshold indices could (quite unexpectedly) be useful for constructing formulas of interpolation character, as shown in the recent paper by Rost and Pattard [20].

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APPENDIX A: EIGENVALUES OF V MATRIX CORRESPONDING TO ROTATIONS AND TRANSLATIONS IN TIME

If the N-particle system is rotated as a whole over an infinitisemal (time-independent) angle $\delta\varphi$ around the axis $\vec{\nu}$, then the particle coordinates receive increments

$$\delta\vec{r}_j^{(\nu)}=(\vec{\nu}\times\vec{r}_j)\,\delta\varphi. \tag{A1}$$

The form of Newtonian equations of motion

$$m_j\frac{d^2\vec{r}_j}{dt^2}=-\frac{\partial U}{\partial\vec{r}_j} \tag{A2}$$

remains invariant under rotations. This implies that

$$m_j\frac{d^2\delta\vec{r}_j}{dt^2}=-\sum_{i=1}^{N}\frac{\partial^2 U}{\partial\vec{r}_i\partial\vec{r}_j}\delta\vec{r}_j, \tag{A3}$$

where $\delta\vec{r}_j=\delta\vec{r}_j^{(\nu)}$. For SC's one can use Eqs. (A1) and (1) to obtain

$$\frac{d^2\delta\vec{r}_j^{(\nu)}}{dt^2}=\frac{1}{\phi}\frac{d^2\phi}{dt^2}\delta\vec{r}_j^{(\nu)}. \tag{A4}$$

Bearing in mind that according to Eq. (18),

$$\phi^2\frac{d^2\phi}{dt^2}=-\frac{\mathcal{Q}_0}{\mathcal{M}} \tag{A5}$$

and using definition (29), we finally obtain

$$\frac{1}{m_j}\sum_{i=1}^{N}V_{ji}\delta\vec{r}_i^{(\nu)}=\frac{\mathcal{Q}_0}{\mathcal{M}}\delta\vec{r}_j^{(\nu)}, \tag{A6}$$

which means that the grand vector $\delta\mathbf{r}^{(\nu)}$ is an eigenvector of the grand matrix $\mathbf{KV}$ with the eigenvalue $\mathcal{Q}_0/\mathcal{M}$. Generally there are three eigenvectors corresponding to this eigenvalue, but for linear SC's only two independent rotations are possible.

Now consider a variation of the trajectory caused by a shifting of time over an infinitesimal interval $t\to t+\delta t$, using a similar technique. For the system in a SC, the particle coordinates are incremented in this case by

$$\delta\vec{r}_j^{(\mathrm{SC})}=\vec{v}_j\delta t=\frac{d\phi}{dt}\vec{\rho}_j\delta t. \tag{A7}$$

The form of Newtonian equations of motion obviously remains invariant under the shift of the time variable. Therefore, Eq. (A3) remains valid for $\delta\vec{r}_j=\delta\vec{r}_j^{(\mathrm{SC})}$. An analogue of Eq. (A4) now reads

$$\frac{d^2\delta\vec{r}_j^{(\mathrm{SC})}}{dt^2}=\left(\frac{d\phi}{dt}\right)^{-1}\frac{d^3\phi}{dt^3}\delta\vec{r}_j^{(\mathrm{SC})}. \tag{A8}$$

Differentiating Eq. (A5), we obtain

$$\frac{d^3\phi}{dt^3}=\frac{2\mathcal{Q}_0}{\mathcal{M}}\frac{1}{\phi^3}\frac{d\phi}{dt}, \tag{A9}$$

which finally brings us to

$$\frac{1}{m_j}\sum_{i=1}^{N} V_{ji}\delta\vec{r}_i^{\,(\mathrm{SC})}=-\frac{2\mathcal{Q}_0}{\mathcal{M}}\delta\vec{r}_j^{\,(\mathrm{SC})}. \tag{A10}$$

Since the grand vector $\delta\mathbf{r}^{(\mathrm{SC})}$ is proportional to the grand vector $\boldsymbol{\rho}$ which defines the SC shape, we conclude that the latter vector is an eigenvector of the grand matrix **KV** with the eigenvalue $-2\mathcal{Q}_0/\mathcal{M}$.

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