

## THRESHOLD BEHAVIOUR OF THE TRIPLE-ESCAPE MOLECULAR FRAGMENTATION FUNCTIONS: I. GENERAL THEORY\*

PETAR V. GRUJIĆ

*Institute of Physics, P. O. Box 57, 11001 Belgrade, Yugoslavia*

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We formulate a general method, within the Wannier classical model, for treating the small-energy molecular fragmentations, with one heavy and three outgoing light particles. Threshold laws for the final configurations of  $C_{3v}$  symmetry have been derived for the pairwise additive potential functions of the inverse-power law and results for the van der Waals interactions are shown. The applicability of the Wannier model has been discussed.

### *1. Introduction*

In a previous paper, to be referred to as I, a method for evaluating threshold behaviour of the double ionization by electrons of atoms and ions has been developed<sup>1)</sup>. The method is based on the classical Wannier's model<sup>2)</sup>, as a generalization of the treatment of double-escape ionization collisions<sup>3)</sup>, within the mathematical formalism first used by Vinkalns and Gailitis<sup>4)</sup>. Essentially the same approach has been used in treating the double ionization by positrons too<sup>5)</sup>. In all these cases the final-state interaction was via the Coulomb force<sup>6)</sup>.

In a recent work it has been shown for the first time that the Wannier's model appears applicable to a more general class of final-state interaction, namely to the molecular breakup processes, when the outgoing atoms interact via non-Cou-

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\* This paper is dedicated to the memory of Professor A. B. Milojević, teacher and friend.

lombic potentials (Grujić and Simonović, to be referred to as II)<sup>11</sup>). The latter work was a generalization of the Coulombic systems triple-escape calculations<sup>7</sup>, to the inverse power-law interactions. Here, we extend the method applied to the triple-escape near the threshold in I, to the case of the interatomic interactions, with the same final-state symmetry configuration  $C_{3v}$ , and for the central body much heavier than the outgoing particles.

In the next chapter we formulate the model for the triple-escape for the four-atom systems, with the pairwise additive inverse-power law interaction potentials. Two special cases: resonant and van der Waals interactions are discussed and treated in the third section. In the appendix A we provide an analysis of the applicability of the classical dynamics in describing the motion of atoms at low energies.

## 2. Threshold behaviour of breakup processes

We shall be interested in the endothermic reactions of the type



where \* denotes the so-called *transition state*, or alternatively, *an activated complex*<sup>8</sup>). Further, we shall be concerned with those situations of collisional dynamics which lead to the final reaction channels with all products possessing individual energies  $E'_i$  much smaller than the endothermicity of the reaction. In this case the fragmentation function threshold behaviour is determined by the outgoing fragments interactions at large separations. (In terms of the chemical kinetics, one speaks then about the so-called *loose transition states*<sup>8</sup>.) Since the small-energy behaviour of the reaction rate of the process (1) is essentially determined by the properties of the very activated complex and not by the way this complex was formed, the entrance channel of the final state from (1) may be one of many possible kinds, like



Of course, the price paid for ignoring the dynamics at the entrance of the reaction, must be the lack of the relevant informations necessary for evaluation of the cross section. Nevertheless, a detailed knowledge of the final-state interaction provides sufficient informations a number of measurable quantities, like the fragmentation threshold law, energy and other distributions etc, to be calculated. In this work we shall be concerned with the first problem — evaluation of the threshold law for the process (1).

### 2.1. Wannier's model

This model, primarily designed for treating processes with purely Coulombic interaction in the final channel<sup>2</sup>, and extended to encompass a wider class of

interactions, see II, is based on a division of the configuration space of the system into two distinct parts: the strong interaction region, where all constituent particles are in close contact, interacting by very complicated forces, and the outer space, where the interaction potential may be described by a pairwise-additive function

$$V = \sum_{i \neq j} C_{ij} / R_{ij}^k, \quad k > 0. \quad (3)$$

Motion within the strong interaction zone (SIZ) is supposed to be sufficiently chaotic a quasiergodic hypothesis to apply<sup>2)</sup>, whereas an accurate description of the system dynamics in the outer region is possible. The outer zone is further subdivided into the so-called *strong-correlations zone* (SCZ), *weak correlations zone* (WCZ) and the *asymptotic zone* (AZ) (see II). It is the boundary between SCZ and WCZ where the loose transient state is eventually formed and where it is decided whether the total fragmentation will take place or not. The system being highly unstable in this narrow region, very accurate description of the system evolution within SCZ is needed, the threshold law to be obtained.

Different theories of the near-threshold fragmentation function behaviour can be formulated within Wannier's model, purely classical, like in II, semiclassical and various quantum-mechanical ones (see, e. g. Ref. 9 for further references). Here we shall adopt what we call the *generalized Vinkalns-Gailitis method*, (GVG)<sup>10)</sup>, based on the Newtonian mechanics. We shall not dwell upon the very applicability of the method to the problem at hand, but direct interesting readers to Ref. II (see also Appendix A).

## 2.2. The leading configuration

As usual, one first determines the subset of all configurations in the final channel that lead to the desired fragmentation at zero total energy  $E$  — so-called *leading configurations*<sup>10)</sup>. To this end, we write the potential energy function of the system in the form

$$V = \sum_{i \neq j} C_{ij} / R_{ij}^k + \sum_{n=1}^3 C_{4n} / R_{4n}^l + W, \quad i, j, n = 1, 2, 3 \quad (4)$$

where the last term in (4) describes the short-range interaction, which may be ignored outside SIZ. Now, guided by the physical considerations, we set up a plane configuration with symmetry  $C_{3v}$  and show that this configuration determines the stationary point on the potential surface, see Fig. 1. With the heavy particle at the origin and light atoms at the vertexes of an equilateral triangle, we write for A-atoms position vectors (see Fig. 1)

$$\vec{r}_l = (r + \Delta_l) \hat{m}_l + \delta_l \hat{n}_l + \nabla_l \hat{k}, \quad l = 1, 2, 3 \quad (5)$$

$$\Delta_l, \delta_l, \nabla_l \ll r, \quad \hat{m}_l \perp \vec{r}_l (\delta_l, \nabla_l = 0), \quad \vec{n}_l \perp \vec{m}_l, \vec{k}, \quad (6)$$

where  $\Delta_l$ ,  $\delta_l$ ,  $\nabla_l$  and are small deviations from the quasiequilibrium positions.

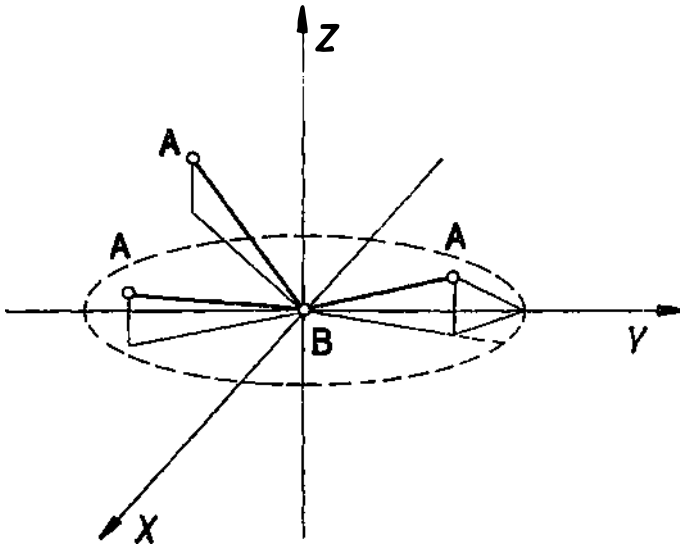


Fig. 1. The perturbed  $B + 3A$  (with symmetry  $C_{3v}$ ) configuration, on the hypersphere  $R = \text{const.}$ , for the case  $B$  much heavier than  $A$ .

We further define the hyper-radius coordinate  $R$  (known also as the giration radius)

$$R^2 = \sum_{i=1}^3 r_i^2 \quad (7)$$

and look for the variation of  $V$  at the hypersurface  $R = \text{const.}$  First, one establishes necessary relationship between the infinitesimal deviations on the hypersphere  $R = \text{const.}$  Inserting Eqs. (5) into Eq. (7), one obtains on the hypersphere the following relation (up to the second order in the deviations):

$$\sum_{i=1}^3 \Delta_i = \frac{1}{2r} \sum_{j=1}^3 (\Delta_j^2 + \delta_j^2 + \nabla_j^2) \approx 0. \quad (8)$$

### 2.3. Perturbed motion

Substituting (5) into (4) and accounting for (8) one has for the potential function near  $C_{3v}$ -symmetry configuration

$$V = \frac{C_{1j}}{2r^k 3^{k/2}} \left( 3 - \frac{k}{2r^2} \sum_i (\Delta_i^2 + \delta_i^2 + \nabla_i^2) + \frac{1}{r^2} O_k(\Delta_1^2, \dots, \nabla_2 \nabla_3) \right) + \frac{C_{4n}}{2r^{kn} 3^{k/2}} \left( 3 - \frac{l}{r^2} \sum_j (\Delta_j^2 + \delta_j^2 + \nabla_j^2) + \frac{1}{r^2} O_l(\Delta_1^2, \dots, \nabla_2 \nabla_3) \right). \quad (9)$$

Hence, we have

$$\frac{\partial V}{\partial \Delta_l} = \frac{\partial V}{\partial \delta_l} = \frac{\partial V}{\partial \nabla_l} = 0, \quad l = 1, 2, 3 \quad (10)$$

$V$  depending quadratically on the small deviations. Further, one can show that the stationary point, determined by (10) is a maximum of (4). This property should be contrasted to that of the Coulombic interaction, see I, and of the collinear configuration, see II, where the stationary points, defined by (10), appear saddle points. Further, from the conservation of the total angular momentum (see I) we have the following constraints

$$\delta_1 + \delta_2 + \delta_3 = 0 \quad (11)$$

$$\nabla_1 = \nabla_2 = \nabla_3. \quad (12)$$

We evaluate now motion along the so-called leading configuration, that is along the individual trajectories which define the potential maximum. In the case at hand, this is a triangular configuration, see Fig. 1, and one obtains in a straightforward manner for  $l = k$

$$\begin{aligned} r^{k+2} &= \gamma t^2 \\ \gamma &= \frac{(k+2)^2}{2m} (C_{14} + C_{13}/3^{k/2}). \end{aligned} \quad (13)$$

Particles moving along the leading trajectories will eventually escape from the central one and from each other. In fact, this to happen (at  $E = 0$ ), it is not necessary all deviations to be at every instance equal zero, but they all should tend to zero in the  $t \rightarrow \infty$  limit.

We assume now that the outgoing particles obey Newton's dynamics (see Appendix A for the corresponding criterion)

$$m_i \frac{d^2 \vec{r}_i}{dt^2} = -k \sum_{j \neq i}^4 C_{jl} (\vec{r}_i - \vec{r}_j) / |\vec{r}_i - \vec{r}_j|^{k+2}, \quad i = 1, 2, 3. \quad (14)$$

Inserting position vectors from (5) into (14), and accounting for the unperturbed motion, one obtains equations for the deviations, within the linear approximation,

$$\begin{aligned} \frac{m_1}{k} r^{k+2} \frac{d^2 \Delta_1}{dt^2} &= \left\{ \frac{1 - 3(k+2)/4}{3^{(k+2)/2}} (C_{12} + C_{13}) - (k+3) C_{14} \right\} \Delta_1 + \\ &+ \frac{1/2 - 3(k+2)/4}{3^{(k+2)/2}} (C_{12} \Delta_2 + C_{13} \Delta_3) + \frac{3(k+2)}{4\sqrt{3}} (C_{12} - C_{13}) \delta_1 + \\ &+ \frac{1}{2} \sqrt{3} \left( 1 - \frac{k+2}{2} \right) (C_{12} \delta_2 - C_{13} \delta_3) \end{aligned} \quad (15)$$

$$\begin{aligned} \frac{m_1}{k} r^{k+2} \frac{d^2 \delta_1}{dt^2} &= \frac{k+2}{4 \cdot 3^{(k+1)/2}} (C_{12} - C_{13}) \Delta_1 + \frac{\frac{k+2}{4} - \frac{1}{2}}{3^{(k+1)/2}} (C_{12} - C_{13}) \Delta_2 + \\ &+ \left\{ C_{14} + \frac{1 - (k+2)/4}{3^{(k+2)/2}} (C_{12} - C_{13}) \right\} \delta_1 + \frac{\frac{1}{2} + \frac{k+2}{4}}{3^{(k+2)/2}} (C_{12} \delta_2 + C_{13} \delta_3) \end{aligned} \quad (16)$$

$$\frac{m_1}{k} r^{k+2} \frac{d^2 \nabla_1}{dt^2} = \left\{ C_{14} + \frac{C_{12} + C_{13}}{3^{(k+2)/2}} \right\} \nabla_1 - \frac{C_{12} \nabla_2 + C_{13} \nabla_3}{3^{(k+2)/2}}. \quad (17)$$

Equations of motion for other two particles are obtained by cyclic permutations of the corresponding indices in Eqs. (15), (16) and (17). We observe immediately that (17) appears uncoupled and can be treated separately from the rest. Making use of the Eqs. (12) one has

$$\frac{d^2 \nabla_1}{dt^2} = \lambda_{\nabla} \frac{\nabla_1}{r^{k+2}}, \quad \lambda_{\nabla} = k C_{14} / m_1. \quad (18)$$

Substituting the unperturbed equation of motion (13) into rhs of (18) we arrive at the Euler equation (accounting again for (13))

$$\frac{d^2 \nabla_1}{dt^2} = \tau \frac{\nabla_1}{t^2}, \quad (19)$$

$$\tau = \frac{-2k C_{14}}{(k+2)^2 [C_{14} + C_{12}/3^{k/2}]} \quad (19')$$

with an immediate solution in the form (we drop the index now)

$$\frac{\nabla}{r} = C_1 r^{\frac{k+2}{4} + \frac{\mu_1}{4}} + C_2 r^{\frac{k+2}{4} + \frac{\mu_2}{4}}, \quad (20)$$

$$\mu^2 = [k^2 + (2 - 8C_{14})^{k+1}] / [C_{14} + C_{12}/3^{k/2}]$$

with  $C_i$  arbitrary constants ( $i = 1, 2$ ).

Writing down corresponding equation for deviations of particle 2 and accounting for the constraints (8) and (11) one arrives at the set of linear differential equations in the matrix form

$$at^2 \frac{d^2}{dt^2} \begin{bmatrix} \Delta_1 \\ \delta_1 \\ \Delta_2 \\ \delta_2 \end{bmatrix} = \begin{bmatrix} F & E & 0 & 2E \\ E & G & 2E & 0 \\ 0 & 2E & F & E \\ -2E & 0 & -E & G \end{bmatrix} \begin{bmatrix} \Delta_1 \\ \delta_1 \\ \Delta_2 \\ \delta_2 \end{bmatrix} \quad (21)$$

\* It might happen that matrix  $A$  can not be diagonalized. Then a special procedure for solving system (21) must be employed (see I).

with ( $C_{14} \equiv C_4$ ,  $C_{1i} \equiv C$ ,  $i = 2, 3$ )

$$\begin{aligned} a &= (k+2)^2 (C_4 + C/3^{k/2})/2k \\ E &= -kC/4 \cdot 3^{(k+1)/2} \end{aligned} \quad (22)$$

$$\begin{aligned} F &= (k+3)C_4 + C/2 \cdot 3^{(k+2)/2} \\ G &= C_4 - 3kC/4 \cdot 3^{(k+2)/2}. \end{aligned} \quad (23)$$

We now rewrite Eq. (21) in the more compact form

$$at^2 \frac{d^2}{dt^2} \underline{\tilde{F}} = \underline{\tilde{A}} \underline{\tilde{F}} \quad (24)$$

and diagonalize\* matrix  $\underline{\tilde{A}}$  by a matrix  $\underline{\tilde{T}}$

$$\underline{\tilde{T}} \underline{\tilde{A}} \underline{\tilde{T}}^{-1} = \underline{\tilde{\Lambda}}. \quad (25)$$

Introducing a new column function  $\underline{\tilde{G}}$  by

$$\underline{\tilde{G}} = \underline{\tilde{T}} \underline{\tilde{F}} \quad (26)$$

one has instead of (24)

$$at^2 \frac{d^2}{dt^2} \underline{\tilde{G}} = \underline{\tilde{\Lambda}} \underline{\tilde{G}} \quad (27)$$

with solution

$$G_i = G_1^{(i)} r^{\eta_1^{(i)}} + G_2^{(i)} r^{\eta_2^{(i)}}, \quad i = 1, 2, 3, 4 \quad (28)$$

$$\eta_{1,2}^{(i)} = \alpha_{1,2}^{(i)} (k+2)/2$$

$$\alpha_{1,2}^{(i)} = \frac{1}{2} + \sqrt{\frac{1}{2} + \frac{\lambda_i}{a}} \quad i = 1, 2, 3, 4. \quad (29)$$

In writing Eq. (28) use has been made of Eq. (13), and  $G_{1,2}$  are arbitrary constants. Now solving back for  $\underline{\tilde{F}}$  in (26) one obtains deviations  $\Delta_1$ ,  $\Delta_2$ ,  $\delta_1$ ,  $\delta_2$  as linear combinations of the exponential functions, which we write in the form

$$\Delta_1/r = \sum_{j=1}^4 T_{1j}^{-1} [G_1^{(j)} r^{\eta_1^{(j)}} + G_2^{(j)} r^{\eta_2^{(j)}}] \quad (30)$$

$$\delta_1/r = \sum_{j=1}^4 T_{2j}^{-1} [G_1^{(j)} r^{\eta_1^{(j)}} + G_2^{(j)} r^{\eta_2^{(j)}}] \quad (31)$$

$$\Delta_2/r = \sum_{j=1}^4 T_{3j}^{-1} [G_1^{(j)} r_1^{(j)} + G_2^{(j)} r_2^{(j)}] \quad (32)$$

$$\delta_2/r = \sum_{j=1}^4 T_{4j}^{-1} [G_1^{(j)} r_1^{(j)} + G_2^{(j)} r_2^{(j)}] \quad (33)$$

$$\varkappa_{1,2}^{(i)} = \eta_{1,2}^{(i)} - 1. \quad (34)$$

Eqs. (30)–(34), together with Eq. (20), determine completely the perturbed configuration. For deriving the threshold law for triple escape, we need further properties of these configurations as function of total energy of the system. These are so-called *scaling transformations*.

#### 2.4. Scaling laws

Let  $\vec{r}_i(t)$  be solutions of Eqs. (14), for a particular value of the total energy  $E$ . If the energy is changed, then all trajectories undergo a homothetic (shape-preserving) transformations<sup>1,2)</sup>

$$r \rightarrow \lambda r, \quad \Theta \rightarrow \Theta, \quad t \rightarrow \lambda^{1+k/2} t, \quad E \rightarrow E/\lambda^k \quad (35)$$

where  $r$  and  $\Theta$  are polar coordinates and  $\lambda$  is a positive real parameter, and  $k$  is defined in Eq. (4), with the homogeneity condition  $k = l$ . From Eq. (5) it follows that all deviations (not necessarily small) transform like  $r$  in Eqs. (35). As we shall see, Wannier's theory makes full use of this fact.

### 3. Derivation of threshold laws

To determine the threshold behaviour of a fragmentation function, we need to know behaviours of the lhs of Eqs. (20) (30)–(34) in the large —  $r$  limit. If any of rhs terms in these Eqs. diverges in the limit  $r \rightarrow \infty$ , the first order perturbation theory breaks, corresponding particle motion deviates considerably from its leading trajectory and merges with another particle of the system. Thus an increasing term signifies a failure of the total fragmentation. The only way to prevent this is to ensure favourable initial conditions, at some initial value  $r = r_0$ , that is sufficiently close to the maximum potential point. The corresponding  $C_i$  constant must be zero for  $E = 0$ , or should assume some small value at  $E$  finite. The larger  $E$ , the larger  $C_i$  value is allowed. Hence, for a fixed  $E$ , there is a maximum numerical value  $C_i^{max}$  which still allows for an infinite motion of the corresponding particle. Obviously as  $E \rightarrow 0$ ,  $C_i^{max}$  must shrink at an appropriate rate. If one assumes that the motion within the sphere with radius  $r_0$  is sufficiently chaotic (quasi-ergodic hypothesis<sup>2)</sup>), then the numerical values of  $C_i$  within the interval  $(0, C_i^{max})$  are uniformly distributed and the total number of the escaping trajectories, emerging from this interval, is simply proportional to the length of the

latter, that is to  $C_i^{max}$ . If it happens that both of terms on rhs of the above Eqs. diverge, the faster is considered only. If neither term grows with  $r$ , the corresponding Eq. is dropped from consideration, since in the limit  $E \rightarrow 0$ , it remains finite.

Now, let there be  $n$  (dominant)  $C_i^{max}$ . Then the part of the corresponding phase space shrinks with decreasing  $E$  as

$$\Delta\Omega \sim \prod_{j=1}^n C_j^{max} \quad (36)$$

(overall probability being the product of single ones). Note that the third particle motion is accounted for via constraints conditions (11) and (8) (the latter with rhs equal zero).

How  $C_i$  depend on  $E$  can be deduced from Eqs. (20) and (30—34) and from the scaling laws (35). Since the lhs must remain invariant, one has an implicate energy dependence of the form

$$C_i \sim E^{\kappa_i/k} \quad (37)$$

and Eq. (36) yields finally the desired threshold law

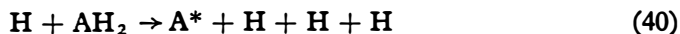
$$\sigma_{fr} \sim E^{\kappa} \quad (38)$$

$$\kappa = \frac{1}{k} \sum_{i=1}^n \kappa_i. \quad (39)$$

Note that for the case at hand, maximum value of  $n$  is 5 (Eqs. (12) impose two constraints). For the molecular systems,  $n$  depends on the actual coupling constants  $C_{ij}$  and  $k$ , as particular  $\kappa_i$  do. We shall now treat two classes of interatomic potential interaction, so-called resonant and van der Waals interactions.

### 3.1. Resonant interaction

This is the case with  $k = 3$ . We distinguish two cases further. (a) The central atom with (almost) resonant interaction with the outgoing particles (the latter assumed to be identical ones). This is the situation with the system



when the excitation threshold for A almost coincides with that for H. The photon moves around from an atom to the other, giving rise to the (quasi) resonant potentials between  $\text{H}^*$  and H:  $V_{HH^*} = \pm 9\sqrt{6}/r^3$ , if the excited state is  $2p^{1,3}$ . The sign of  $V$  depends on the magnetic quantum numbers of  $2p$  orbitals. Similarly with  $\text{A} + \text{H}^*$  interaction.

We note that in the case of four H atoms, when the interaction is of pure resonance type, the present theory is invalide, first since the central body is not much heavier than the outer ones, and second the leading configuration might be different from the one adopted here.

b) The central atom does not support (quasi) resonant interaction. In that case an oscillatory-like interaction between the middle body and the rest appears, with the potential decreasing with distance as inverse square, or inverse fourth power law<sup>13)</sup>. These interesting phenomena deserve a particular attention and shall be treated in a future investigation. Note that the same sort of interaction arises when two or more atoms are in excited states at the same time.

### 3.2. Van der Waals interaction

If all atoms remain in the ground states in the final channel, dominant long-range interaction is of the van der Waals kind, i. e.,  $k = 6$ . The threshold exponent is a function of the relative strength of the corresponding coupling constants  $C_4$  and  $C$ . If the first may be neglected, one has from (38), (39)

$$\sigma_{fr} \sim E^{2.0365}. \quad (41)$$

Whether this particular threshold behaviour really holds, depends on the very applicability of the classical model. This must be examined beforehand. We present in the Appendix A some general analysis for a number of inverse-power law interactions.

Generally, nonadditive three-body forces may be present in the final channel, but they fall off much faster than the dipole terms, and can be neglected (see, e. g. Ref. 14 and references therein). The same applies even more for the exponentially decreasing exchange interactions.

### Acknowledgements

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## APPENDIX A

### *The classical approximation*

For an applicability of the (semi) classical theory, one requires that de Broglie wavelength of a moving particle

$$\lambda = \hbar/p$$

does not change significantly over a characteristic length, which requirement may be cast into the formal condition

$$F(r) \equiv |d\lambda/dr| \ll 1. \quad (A.1)$$

For a finite particle energy  $E$  and the potential of the form  $Cr^{-k}$  (A.1) takes the form (see Fig. 2)

$$F(r) = k|C|(E - Cr^k)^{-3/2} r^{-k-1} / \sqrt{8m}. \quad (A.2)$$

For sufficiently small or large  $r$ , (A.1) will be satisfied. We seek, however, conditions which ensure formation of the wave packet across the entire configuration space. Function (A.2) has a maximum

$$F_m = F(r_m) = \frac{2^{1/k} (k-1)^{1+1/k} (k-2)^{1/2-1/k}}{3^{3/2} \sqrt{2km} |C|^{1/2} E^{1/2-1/k}} \quad (\text{A.3})$$

at

$$r_m = \left\{ \frac{C(2-k)}{2E(k+1)} \right\}^{1/k}. \quad (\text{A.4})$$

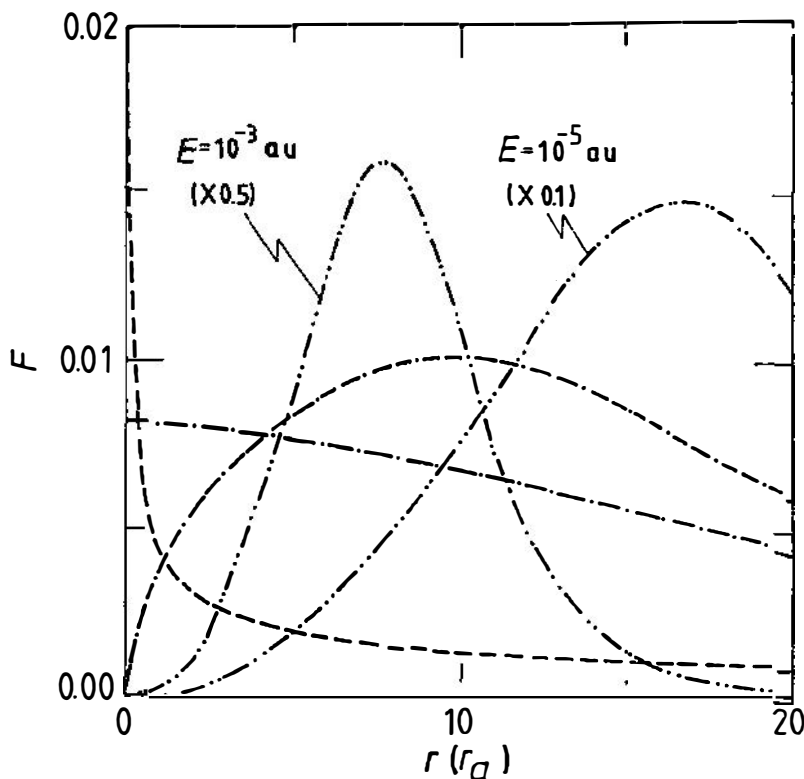


Fig. 2. The plot of the function (A.2) for some characteristic  $k$ -values. (Note the change of scale). Curves are given for appropriate (small) values of the energy  $E$ , and coupling constants  $C$ .  $k = 1$ : ----, ( $C = 0.75$ );  $k = 2$ : - · - · - ( $C = 0.75$ );  $k = 3$ : - · - · - · - ( $C = 7.5$ );  $k = 6$ : · · · · · ( $C = 750$ ). In all cases the mass of an interacting atom is  $m = 10^4$  au and  $C$ -values are in au.

As  $E$  tends to zero,  $r_m$  increases, as  $F_m$  does, and for a sufficiently small  $E$  a »quantum mechanical barrier« appears. However, the relation  $F_m \ll 1$  is a sufficient, but not a necessary condition for applying the classical model. As shown by Wannier, it is the region bounded by  $R$  (Wannier's radius), where it is decided whether the double escape will take place or not. Hence, once all particles separate from

each other sufficiently enough their motion towards the truly free zone may be described in whatsoever manner. From (A.2) we see that in the limit  $r \rightarrow 0$  both  $F(r)$  and  $dF/dr$  tend to zero as well, but this fact is of little practical significance for the atomic, that is finite, systems. Once the atomic dimensions are fixed up, it is the height and position of  $F_m$  which is critical to the classical approximation.

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## PONAŠANJE MOLEKULARNIH FRAGMENTACIONIH FUNKCIJA ZA TROSTRUKI BEG U BLIZINI PRAGA: I. OPŠTA TEORIJA

PETAR V. GRUJIĆ

*Institut za fiziku, P. P. 57, 11001 Beograd, Yugoslavia*

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Formulisana je opšti metod, u okviru klasičnog Vanieovog modela, za opisivanje molekularne fragmentacije pri malim energijama, sa jednom teškom i tri odlazeće lake čestice. Zakon praga za krajnju konfiguraciju  $C_{3v}$  simetrije izveden je za slučaj poparno aditivnih potencijalnih funkcija sa inverznim stepenim zakonom i dati su rezultati za van der Valsove interakcije. Diskutovana je primenljivost Vanieovog modela.