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## THRESHOLD ESCAPE OF TWO ELECTRONS AND CONNECTIONS TO AUTOIONIZING STATES

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Résumé. - L'ionisation double de l'atome neutre près du seuil de ce processus met en jeu de très fortes corrélations radiale et angulaire entre les deux électrons. Le traitement détaillé de ces corrélations est nécessaire pour reproduire le comportement près du seuil de la section efficace d'ionisation double. Les états doublement excités des atomes au-dessous du seuil présentent des comportements similaires. La localisation de la fonction d'onde dans une région où il n'existe pas de manière évidente de potentiel de liaison joue un rôle important dans ces deux situations. Des mécanismes analogues existent lors du mouvement hautement corrélé de l'électron de faible énergie soumis à l'action combinée d'un champ coulombien et d'un champ statique extérieur, magnétique ou électrique. Les similarités entre ces divers phénomènes sont soulignées au cours de la discussion détaillée de la double ionisation.

Abstract. - The escape of two electrons from a positively charged core just above the threshold for this process involves strong radial and angular correlations between them. Careful treatment of these correlations is needed to derive the threshold behavior of the cross-section for such double escape. Doubly-excited states of atoms below the threshold also involve the same kind of correlations although to a different degree. There are, therefore, close connections between the two problems. A localization of the wave function into a region where there are no obvious binding potentials plays an important role in both phenomena. Similar localization is also involved in the highly correlated dynamics of a single electron of low energy moving in combined Coulomb and external magnetic or electric fields. Through a detailed discussion of threshold double escape, the connections between these various phenomena are highlighted.

## I. Introduction

The subject of atomic ionization in which an initial event leads to two slow electrons escaping from a positively charged core is of basic and fundamental interest by virtue of the very subtle dynamics involved. This problem of "threshold double escape" bears on the other problems of highly correlated motion that are of interest to this workshop, namely the study of high Rydberg states of atoms in external fields and the study of doubly-excited states of atoms. Many features of the physics and mathematics of the phenomena are common to all these problems.

In studying single electron excitation, it has become customary to view the entire set of discrete singly-excited states and the ionization continuum as part of the same family. In particular, the recognition that there is an intimate connection between the highly discrete states and the region just above the threshold for single ionization, as exemplified by the equality between the

quantum defect (in radians) and the zero energy phase shift, is the basis of the very successful quantum defect theory [1][2]. Exactly similarly, doubly-excited states of atoms and the two-electron continuum are viewed together with advantage and the study of both parts is a necessary ingredient for the development of two-electron quantum defect theory [3][4].

In particular, I wish to emphasize here that in the connection between two-electron states above and below the threshold for double escape, the state exactly at threshold plays a crucial role. It serves as a kind of "parent state", exhibiting correlations and other aspects of two-electron dynamics at their most pronounced level. These effects remain in the other states connected to this parent state at  $E=0$ , the high-lying doubly-excited states (at  $E \leq 0$ ), with both electrons having large principal quantum number, and the low energy two-electron continuum ( $E \geq 0$ ) which is crucial for the understanding of electron-atom scattering in this "intermediate energy" region. The correlations trail off with increasing  $|E|$  although they remain largely relevant even down to the lowest members of the manifold of doubly-excited states. [In negative ions, even the ground state shows a fairly high amount of such correlations which are responsible for the very stability of the system--the canonical example is radial correlation in  $H^-$ .] That the threshold for double escape has a special status with regard to such correlations is understandable because the two electrons are slow and there is a long time for interaction as they escape to infinity. The angular and radial correlations that are already familiar in doubly-excited states are at an extreme for the threshold state. As a result, the study of threshold double escape is very well-suited for understanding these correlations, particularly given that threshold laws focus on long range interactions (See the sketch in sec. II. below, also sec. II of [5]).

The feature of a special, highly correlated state playing the role of a parent state for other states which exhibit similar correlations to a lesser degree occurs elsewhere in physics as well. The most prominent examples are ground states of nuclei containing many nucleons or, more generally, plasma modes or superconducting states in many-body systems. Low-lying quasiparticle excitations from such a highly correlated state can be viewed as a family of states built on the parent state. Interestingly, in all such examples the highest correlation is seen in the ground state of the system so that the study concentrates on low energy excitations. In atomic physics on the other hand, because the two-particle interaction is repulsive and not attractive as in the other examples, the strongest correlations are not to be seen in ground states of atoms but rather higher in energy at the double escape threshold [6].

A second striking feature of the behavior near the double escape threshold and its contact with other physical phenomena is that the highly correlated state is localized in a limited region of configuration space. Once again, this is already clear from the study of doubly-excited states where basic features such as their high metastability are understood in terms of the concentration of their wave function into regions of configuration space quite different from where the states of single excitation or ionization lie, resulting in little overlap between them [7]. An understanding of this localization is gradually emerging particularly with connections to similar phenomena in the study of high Rydberg states in external fields [8][9]. This study, of central interest to this workshop, has shown that quite generally one sees characteristic broad resonances near the single ionization threshold when an atom is placed in an external electric or magnetic field. (See the other contributions to this workshop and references in recent reviews [10]). The problem of threshold double escape constitutes a highly

correlated motion of two electrons in the field of an ion core whereas the external field problem involves the correlated dynamics of a single electron in the presence of two competing external fields. In both cases there seems to be a localized mode concentrated in a metastable region of the potential, a "ridge" of the potential [8]. The mathematical physics of these problems has, therefore, much in common. Note also that in both cases the phenomena are associated with a near-threshold energy region where there is a very high density of states. WKB methods and even classical trajectory calculations have therefore, played a major role in the development of our understanding of all these phenomena [10]. More broadly, all these problems represent the study of the motion of a configuration point in a non-separable potential, particularly near saddle points of the potential, so that certain directions of motion correspond to stable or bound-state characteristics and others to unstable or escape behavior [11]. This results in strongly correlated phenomena such as fairly narrow resonances and in the threshold behavior to be discussed below.

## II. Threshold Laws, Diagnostics for Long Range Interaction

A crucial feature of the study of the energy dependence of a reaction cross-section just above the threshold for the process, emphasized from the very beginnings of such studies [12], is that the threshold behavior depends only on the escape process. Details of the initial event that created such an escape configuration (for instance, the nature of the impact, whether by photons or electrons) or what goes on in the complicated inner zone (the "reaction zone") when all particles are close together and interacting strongly, are largely irrelevant. Instead, the question is, given the emergence of the escaping particles at  $r_0$ , the boundary of the reaction zone, with enough energy  $E \geq 0$  to escape to infinity, what in the subsequent evolution will determine the probability that they do in fact reach infinity. One implication of this is that in the absence of any interactions between the particles outside the reaction zone, the threshold law is given simply by the available phase space for the escaping particles. More importantly, a second implication is that the escape near threshold is sensitive only to the longer range interactions that prevail outside the reaction zone and it is this region of weak forces that can introduce strong dependences on  $E$ . Threshold laws are, therefore, the natural objects of study if we wish to understand the influences of long range forces and correlations clearly separated from the shorter range interactions between particles.

To collect a few representative examples of canonical threshold laws [12], we start with the simplest when one particle separates from the rest and only short range interactions are involved. The phase space factor,  $k^2 dk/dE$ , where  $k = (2Em/\hbar^2)^{1/2}$  is the wave-vector, gives  $\sigma \propto k$ . Examples are legion in many areas of physics when a reaction such as photo-detachment of a negative ion leads to an escaping particle with angular momentum  $\ell=0$ . By contrast, when a long range potential is present as, for instance, if the escape is into a  $\ell \neq 0$  partial wave, the threshold law is modified to  $\sigma \propto k^{2\ell+1}$ . The repulsive long range angular momentum potential suppresses the threshold law. Stated quantitatively, the wave amplitude at small  $r$  near  $r_0$  is lowered by a  $r^\ell$  factor which results in a weighting of the probability by  $k^{2\ell}$ . If, instead, the escape involves a long range attraction like the Coulomb potential as in photo-ionization of a neutral atom then the wave function density is enhanced at small  $r$  by the Coulomb enhancement factor [13],

$$|\Psi(0)|^2 \propto [k(1-e^{-2\pi/k})]^{-1} \propto k^{-1} . \quad (1)$$

Therefore, the phase space result is now enhanced to  $\sigma \propto k^0$ , that is, the cross-section is finite and constant at threshold.

Turning to many-particle escape in the presence of purely short range forces, one needs only to account for the phase space factors for each particle. Thus, when two particles escape from a residual core, one has

$$\sigma \propto \iint dE_1 dE_2 \delta(E-E_1-E_2) (k_1^2 dk_1/dE_1) (k_2^2 dk_2/dE_2) \propto E^2 , \quad (2)$$

where the integrations and delta function enter because one has to sum over all possible partitions of the available energy  $E$  into the individual energies,  $E_1$  and  $E_2$ , of the escaping particles. To set the stage for the next section, departures of the threshold exponent from 2 will reflect enhancements or suppressions owing to the long range interactions between the escaping particles.

### III. Double Escape of Two Electrons

For the examples considered in sec. II, specifics of the wave function of the final escape state were either not required (phase space alone sufficed) or, when required as in (1), were unambiguous. When we turn to multiple escape with long range interactions, the description of the final state is non-trivial. The rest of this paper concerns itself with threshold double escape when as a result of photo double-detachment of a negative ion or electron impact ionization of a neutral atom, there results the configuration  $\rightarrow A^+ + e + e$ . There is now a long range Coulomb interaction between all pairs. From the discussion in sec. I, we can expect that a description of the two-electron final state in terms of independent particle pictures will be inadequate. Specifically, note that were we to consider the wave function as a product of Coulomb waves implying that each electron sees some fixed, partially screened nuclear field due to the presence of the other, there enter into the integrand in (2) the factors  $1/k_1$  and  $1/k_2$  from the Coulomb wave function density as given in (1). This would enhance the threshold cross-section to a linear law  $\sigma \propto E$ . On the other hand, an alternative picture of the screening in terms of an inner electron seeing the Coulomb field of the core but the outer seeing an overall neutral field would lead to only one such factor from (1) and the result  $\sigma \propto E^{3/2}$ . Thus, the threshold law depends on the assumptions made about the mutual screening during the escape process. All such descriptions in terms of some 'static' screening and a final state function expressed as a product of wave functions for the two electrons are grossly inadequate. They fail to take into account the strongly correlated nature of two-electron states which was emphasized in sec. I. We know from the study of doubly-excited states that any such description of them in a single particle picture involves a superposition of many configurations and the superposition gets larger with increasing excitation. Right at the double escape threshold, therefore, such a superposition fails qualitatively. We turn, therefore, to one particular theory of double escape, the Wannier theory [5][14], which departs completely from single particle pictures and emphasizes throughout the inherently two-electron character of the escape channel.

The Wannier Theory. That the final state of double escape involves strong correlations between the electrons is exemplified by the following description [5]. For simplicity, we begin with a two-electron configuration in  $1S_0$ . The extension to non-zero total orbital and spin angular momentum will be taken up in sec. IV. The two-electron  $1S_0$  state can be completely described by three coordinates  $r_1$ ,  $r_2$  and  $\theta_{12}$ , the two radial distances and the angle between the unit vectors  $\hat{r}_1$  and  $\hat{r}_2$ , respectively. In a time-dependent picture of the escape process outside the reaction zone, consider at some instant that E is partitioned into  $(E_1, E_2)$ . This translates through the speeds of the two electrons into a corresponding set of values for  $r_1$  and  $r_2$ . Consequently, each electron screens part of the Coulomb field of the core for the other and there is a resulting energy exchange between them leading to a new set of  $(E_1, E_2)$  for the next instant. The entire escape process can, therefore, be pictured as a sequence of such snapshots, with the configuration at any instant determining the screening and thereby the partitioning of E leading to the next configuration. The screening is, therefore, intrinsically dynamic in character, an energy-dependent screening which cannot be cast in the form of some static values fixed for the entire escape. The picture also suggests the crucial role played by the ratio  $r_1/r_2$ , the variable for radial correlations between the two electrons. In fact, a slightly deeper look at this dynamic screening brings out even more the importance of this ratio because departures of this ratio from unity are inherently unstable. The slower electron, in hanging back closer to the nucleus, screens its field more making the faster one even faster. Thus any initial discrepancy in the values of  $r_1$  and  $r_2$  or, correspondingly,  $E_1$  and  $E_2$ , is magnified; exactly at threshold, when there is a large time for evolution of the state towards escape, there is a significant probability of the slower electron losing so much energy as to end up trapped onto the core. This can also be stated alternatively that just near the double escape threshold, the two-electron continuum is degenerate with an infinite number of single ionization continua representing one of the electrons bound into a Rydberg state; all these channels represent the possibility of a loss of flux from the double escape channel. In terms of the potential, the two-electron potential exhibits a ridge at  $r_1 = r_2$  which separates deep valleys at  $r_1 \gg r_2$  and  $r_2 \gg r_1$ .

The above description pointing to the crucial importance of  $r_1/r_2$  staying close to unity for a large part of the escape if double escape is to result singles out a region of two-electron configuration space as of special importance. Given the general conjugate relationship in quantum mechanics between state space and configuration space it also points to the necessity in single particle descriptions to superpose a large number (infinite) of states in order to construct such a tightly constrained wave function that maintains  $r_1/r_2 \approx 1$ .

The necessity for superposing many configurations, already known for low lying doubly-excited states, is seen, therefore, to become particularly acute in the vicinity of the double escape threshold. Next, the discussion also points to a natural choice of coordinates for describing these highly correlated situations, namely, that  $r_1/r_2$  is a more appropriate variable for radial correlation than the independent particle coordinates  $r_1$  and  $r_2$ . In terms of an angular

variable to handle correlations, just as angular correlations are described by  $\theta_{12}$ , one defines a hyperspherical "angle"  $\alpha = \tan^{-1}(r_2/r_1)$  for the radial correlations. Together with the hyperspherical radius  $R = (r_1^2 + r_2^2)^{1/2}$ , the double escape wave function is more appropriately viewed in  $(R, \alpha, \theta_{12})$  than in  $(r_1, r_2, \theta_{12})$ .

The passage from Cartesian to circular coordinates in the  $(r_1, r_2)$  quarter plane ( $0 \leq \alpha \leq \pi/2$ ) is by now also familiar from the study of doubly-excited states in hyperspherical coordinates [15]. There too the primary motivation for using  $\alpha$  and  $\theta_{12}$  is that when the correlations between the two electrons are important one should view  $\psi(\vec{r}_1, \vec{r}_2)$  not in terms of products of single particle wave functions but directly as a two-electron wave function. In terms of  $\alpha$  and  $\theta_{12}$  the radial and angular correlations are cleanly separated. We will see in what follows that this separation is also very useful because the two kinds of correlations have qualitatively different roles to play in double escape.

Two two-electron potential in  $(R, \alpha, \theta_{12})$  exhibits at any  $R$  a saddle point at  $(\alpha = \pi/4, \theta_{12} = \pi)$  with deep valleys at  $\alpha \simeq 0$  and  $\pi/2$  and peaks at  $\alpha = \pi/4$  and  $\theta_{12} \simeq 0$  and  $2\pi$ [5][14]. [See figures in [3] and [5]]. The ridge at  $\alpha = \pi/4$  has already been mentioned. With regard to  $\theta_{12}$ , there is a natural tendency for the configuration point to move down to  $\theta_{12} \simeq \pi$ , that is, for the two electrons to end up at  $\hat{r}_1 = -\hat{r}_2$  as a result of their repulsion, particularly near threshold when the electrons are slow. In this manner, a specific region of the two-electron configuration space, the region around the saddle point, is singled out as of critical importance for double escape [14]. The wave packet resides in this region for a large part of the escape, that is, till  $R$  attains large values. The particularly non-trivial aspect of this localization is in the  $\alpha$  coordinate because this region is the top of a ridge of the potential. An understanding in detail of such a localization at a ridge has yet to be worked out but several pieces of evidence have emerged which I will discuss here. Evidence for such concentration of the wave function into the saddle-point region is provided by hyperspherical studies of doubly-excited states [15]. Such states have been grouped into various families according to a quantum number of radial correlation (denoted by  $m$  or  $n_{rc}$ , the generalization of the initially introduced  $\pm$  quantum number), which measures the number of nodes in  $\alpha$ . In particular, states with nodes at the ridge behave very differently from those which have an antinode there and the one with largest amplitude there is the one that carries the most intensity as seen in experiments. The precise tracing of the connection between members of like families (or whether this also goes across families) with increasing excitation and the final connection to the state at threshold remains to be developed. The picture of a localization at a ridge of the potential is also successful in the study of high Rydberg states in external fields in accounting for the broad resonances seen right around the Rydberg limit. The combined Coulomb and magnetic potential  $-1/r + \frac{1}{8} B^2 r^2 \sin^2 \theta$  exhibits a ridge at  $\theta = \pi/2$ . Confinement along the ridge accounts for the resonances seen [10]. There too, detailed treatments of such localization at a ridge are only just beginning [8]. See in particular recent treatments of an atom in a magnetic field [9].

To examine further the behavior in the vicinity of the saddle point in the two-electron problem, let us first look [5] at the potential (in a.u.) expanded into  $\beta \equiv \pi/4 - \alpha$ ,  $\gamma \equiv \pi - \theta_{12}$ :

$$V(R, \alpha, \theta_{12}) = (-Z_0 - Z_\alpha \beta^2 + Z_\theta \gamma^2)/R, \quad (3)$$

$$Z_0 = 2\sqrt{2}(Z - 1/4), \quad Z_\alpha = 3\sqrt{2}(Z - 1/12), \quad Z_\theta = \sqrt{2}/16. \quad (4)$$

Thus in the region of the saddle there is a harmonic oscillator potential in  $\gamma$  and one with opposite sign in  $\beta$  (top of a ridge). The kinetic energy in the saddle takes the form [5]

$$T = -\frac{1}{2} \left\{ \frac{\partial^2}{\partial R^2} + \frac{1/4}{R^2} + \frac{1}{R^2} \left[ \frac{\partial^2}{\partial \beta^2} + 4 \frac{\partial^2}{\partial \gamma^2} + \frac{4}{\gamma} \frac{\partial}{\partial \gamma} \right] \right\}. \quad (5)$$

Near zero energy, solutions of the two-electron Schrödinger equation  $(T+V)\phi=0$  can be found [5];

$$\phi(R, \beta, \gamma) = \chi(R) \exp[icR^{\frac{1}{2}} + \frac{1}{2}iac\beta^2 R^{\frac{1}{2}} - bc\gamma^2 R^{\frac{1}{2}}], \quad (6)$$

where  $a, b$  and  $c$  are constants dependent on  $Z$ . In particular, two alternative values of  $a$  obtain with [5]

$$a = (-1 \pm 2\mu)/8, \quad \mu = \frac{1}{2}[(100Z-9)/(4Z-1)]^{\frac{1}{2}}. \quad (7)$$

In arriving at (6) and (7), the coupling between the motion in  $R$  and in the hyperspherical angles is critical and contrasts with the adiabatic separation between them which obtains [15] for low-lying doubly-excited states. We note that these solutions are obtained through a WKB approximation or variants thereon [5]. Similarly, the non-separable motion for a high Rydberg state in an external field involves a WKB procedure typically involving two variables in place of the three here [11].

The two values of  $a$  in (7) correspond to wave functions or, correspondingly, quasi-classical trajectories that either converge to or diverge from the ridge. The occurrence of alternative signs for the gradient of the phase in (6) is not surprising because in the balance between  $T$  and  $V$  in the Schrödinger equation, the former involves only the square of this gradient. The diverging trajectories in particular represent the anticipated loss of flux from the saddle point region. Either in terms of trajectories [14] or an energy dependent weight factor as in (1) for the squared wave function derived [5] from (6), one obtains for the threshold law for double escape

$$\sigma \propto E^{\frac{1}{2}\mu - \frac{1}{4}}. \quad (8)$$

This is the Wannier threshold law,  $\sigma \propto E^{1.127}$  when  $Z = 1$ . That the exponent is slightly larger than 1, the result pointed out in sec. II in the absence of the electron-electron interaction, is a reflection of the long range radial correlations and the associated instability leading to a suppression of the threshold cross-section. The  $Z$  dependence of the exponent is also perfectly natural because dynamic screening involves a competition between the electronic repulsion and the  $Z$ -dependent attraction of the core. Finally, unlike the motion in  $\alpha$ , the motion in  $\theta_{12}$  is stable, and does not upset the development of a double escape configuration and, therefore, does not influence the threshold exponent [5][14]. Other aspects of the angular correlation will be discussed in sec. IV.

To connect these considerations of the saddle region with doubly-excited states note from (3) and (5) that there are bound state solutions of this 6-dimensional problem. In fact, if the terms in  $\beta$



and  $\gamma$  in (3) are dropped, we have simply a Coulomb potential  $-Z_0/R$  in 6-dimensions with eigenvalues

$$E_n = -\frac{1}{2} Z_0^2 / (n+5/2)^2, \quad n = 0, 1, \dots \quad (9)$$

High doubly excited states with main concentration in the saddle can then be identified as bound below the double escape threshold with the energy in (9), with a modification of  $Z_0$  by the effect of the motion in  $\beta$  and  $\gamma$  in (3). Read et al. [16] have, semiempirically carried out such fits with a non-integral charge and the fits account quite well for a number of doubly excited states of atoms and negative ions. The picture I wish to emphasize here based on (3) and (5) is that one can analyze such data for evidence of the localization in  $\beta$ . Note first that quantizing the motion in  $\gamma$  in (3) and (5) into its lowest state leads to an effective reduction of the charge  $Z_0$ . On the other hand, the "anti-oscillator" in  $\beta$  will modify  $Z_0$  by adding a complex quantity to it. The imaginary part will, of course, be associated with the width of such doubly-excited states, the auto-ionization width into the single escape channels. The real part, if it enhances  $Z_0$  and thereby the binding in (9), will be evidence for localization in the motion away from the saddle in the  $\beta$  direction.

#### IV. Energy and Angular Correlations and Extensions to General L and S

The Wannier theory discussed in sec. III not only gives the threshold law for double escape in (8) but is rich in the connections to doubly-excited states and in the detailed statements about the correlations between the two electrons. To expand on this further, note that already even in the  $^1S$  configuration, the confinement to a small range of  $\alpha$  and  $\theta_{12}$  means the superposition of a large number of the corresponding angular harmonics. In terms of the angles  $\hat{r}_1$  and  $\hat{r}_2$ , the restriction to  $\hat{r}_1 \simeq -\hat{r}_2$  implies a superposition of a large number of large  $\ell$  values for each electron. This has been noted [5] and its experimental realization has been discussed [17]. Also the importance of such a superposition of  $(\ell_1, \ell_2)$  is known from the hyperspherical [15] and group-theoretic [18] classification of doubly-excited states. Thus most of the essential features of radial and angular correlations are already contained in the  $^1S$  description. Also, as in general for any Coulomb threshold law, effects of higher L are not expected to change the threshold law as such because of the overwhelming dominance of a  $1/R$  potential over  $1/R^2$ . However, the extension of sec. III to general L, S, and  $\pi$  (parity) of the outgoing electrons is of interest because of the further influence on some of the correlations. In particular, since a special symmetric configuration,  $\hat{r}_1 \simeq -\hat{r}_2$ , plays an important role, aspects of the Pauli principle for two electrons in some  $\{L, S, \pi\}$  may be expected to be of interest.

Here, the different roles of  $\alpha$  and  $\theta_{12}$  in the Wannier theory is crucial [19]. As we have seen, the crucial element is the unstable coordinate and that it be possible to maintain the configuration  $r_1 = r_2$ . The two electron wave functions must, therefore, be symmetric under purely radial interchange  $r_1 \leftrightarrow r_2$  or  $\beta \rightarrow -\beta$  as is (6). On the other hand, for even parity states of  $L=0$  and 1 which can only be constructed from  $\ell_1 = \ell_2$ , there are two states  $^3S^e$  and  $^1P^e$  which are symmetric under the interchange of spin coordinates and  $\hat{r}_1 \leftrightarrow \hat{r}_2$ . For

the overall wave function, the requirement of antisymmetry under particle interchange requires, therefore, that it be antisymmetric under radial interchange, that is, that it have a node at  $r_1 = r_2$ .

This leads [19][20] to a further suppression of the double escape, such an overall multiplicative factor in  $\beta$  in (6) giving rise to a much higher threshold exponent in (8), namely 3.88 for  $Z=1$ . The above statements regarding the two-electron wave function in  $^3S^e$  and  $^1P^e$  are also relevant for doubly-excited states and it is known [15] that they have a node at the ridge  $\alpha = \pi/4$ . As a corollary, the  $^1S^e$  and  $^3P^e$  always have an antinode at that point. For any other values of  $\{L, S, \pi\}$ , the spatial wave function  $\psi_{LS\pi}$  does not have definite symmetry under the radial interchange  $r_1 \leftrightarrow r_2$  but can always be written as

$$\psi_{LS\pi} = \psi_{LS\pi}^{(+)} + \psi_{LS\pi}^{(-)} \quad (10)$$

The two parts are respectively symmetric and antisymmetric under  $r_1 \leftrightarrow r_2$  or  $\beta \rightarrow -\beta$ . As regards the threshold law, the + function exhibits the exponent 1.127 and the - the more suppressed 3.88 so that it is the + state that controls the threshold behavior. Thus nearly all  $\{L, S, \pi\}$  exhibit the Wannier threshold law for double escape. Further, in a situation such as electron impact ionization of an atom where the threshold double escape gets contributions from various L and S, the cross-section for triplet and singlet ionization will have the same energy dependence. Recent experiments [21] with spin-polarized electrons on polarized atoms bear this out. Also, since all the + states share the behavior in the  $\alpha$  coordinate discussed in sec. III, the energy correlations between the electrons will be the same for all  $\{L, S, \pi\}$ . Note from the squared wave function in (6) that there is no  $\beta$  dependence--all possible ratios  $E_1/E_2$  are equally likely [22] [23]. Experiments which have verified the Wannier threshold exponent of 1.127 have at the same time borne out this result for the mutual energy distribution between the outgoing electrons [24][25]. The central feature of the Wannier theory, that equal partition of the energy between  $E_1$  and  $E_2$  is as likely as any other, seems to be valid for E values up to a couple of eV above threshold [25].

The main difference between the + states in (10) in double escape lies in the angular aspects [19]. Note first of all from (6) that for the  $^1S$  state, the squared wave function is a gaussian in  $\gamma$ . More quantitatively, one can show [23] that it implies that the electrons emerge into a cone with  $\hat{r}_1 = -\hat{r}_2$  and that the width of this cone increases proportionally to  $E^{3/4}$ . With some remaining discrepancy in the numerical pre-factor, the one experiment [24] which measured the escaping electrons in coincidence has indeed verified the  $E^{3/4}$  dependence. On the other hand, the angular distribution can be quite different in other  $\{L, S, \pi\}$  states. Note first that under  $\hat{r}_1 \leftrightarrow \hat{r}_2$  interchange, the spatial wave function  $\psi_{LS\pi}$  acquires a  $(-)^S$  sign. Also, under the parity operation, we have  $\psi_{LS\pi}(-\hat{r}_1, -\hat{r}_2) = \pi \psi_{LS\pi}(\hat{r}_1, \hat{r}_2)$ . At the saddle ( $\vec{r}_1 = -\vec{r}_2$ ) therefore, the combined operation of interchanging  $\vec{r}_1$  and  $\vec{r}_2$  and reflection shows that the wave function must vanish if  $\pi(-)^S$  equals  $(-1)$ . Thus a general  $\psi_{LS\pi}^{(+)}$ , even while having no node in the  $\alpha$  coordinate at the ridge and thereby exhibiting the exponent 1.127, may nevertheless be vanishingly small in amplitude

there. This must result from an angular node. As a specific example, this is easily seen for  $^1P^0$ , a state of importance because it is the one reached in photo double detachment of  $H^-$  and where recent experimental data [26] is consistent with the Wannier law. The symmetry of this state is that of  $\tilde{\chi}_1 + \tilde{\chi}_2$  which vanishes at the saddle by virtue of the angular part of the function. First of all this means that the cross-section in such channels is necessarily small because of the smallness of the proportionality coefficient in (8). This is a "dynamical forbiddenness", noted in another context [27] for  $^1P^0$  doubly-excited states. Next, the angular behavior in  $\theta_{12}$  is quite different in such an  $\{L, S, \pi\}$  than in  $^1S$  with in fact a zero for  $\theta_{12} = \pi$ . One can show [19] that in such a photo double detachment of  $H^-$ , if one measures only one of the escaping electrons with respect to the polarization of the photon, this zero at  $\theta_{12} = \pi$  translates into a  $\sin^2\theta$  angular distribution. Again, this connects to what has been noted for the photoelectron angular distributions on the other side of threshold, that in photo detachment of  $H^-$  with simultaneous excitation to  $H(n)$ , such a  $\sin^2\theta$  distribution obtains as  $n$  gets large [27]. Finally, we note once again as a connection to doubly excited states that the division in (10) into  $\pm$  states and its specific realization in these angular aspects (that under angular interchange they acquire a factor  $\pm(-)^S$ ) makes contact with the study of angular correlations in the  $O_4$  group classification of doubly-excited states [18]. The quantum number  $T$  alternates precisely in this manner for singlet and triplet states.

In summary, the threshold double escape of two electrons from an ion has a good claim to be the premier example of correlated dynamics in atomic physics and its study bears on a number of other phenomena of strongly correlated motion.

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