THE THRESHOLD LAWS FOR ELECTRON-ATOM AND POSITRON-ATOM IMPACT IONIZATION

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Introduction and Summary

In view of the fact I have long been interested in the electron-atom impact ionization problem, and have published several papers on it over the years,^{1,2} I would like in this talk to review only the most salient aspects of my work, which has only recently culminated with what I believe is a derivation of the correct threshold law.³ By way of introduction let me emphasize that because the problem deals with three separating charged particles at the lowest energy at which they can escape from one another, this is the most basic three-body problem in the continuum involving Coulomb (i.e., long-range) forces. At the same time it also involves quantum mechanics in a very fundamental way, in my opinion.

What I would like to do here is to emphasize, schematically through a series of figures, aspects of my approach -- the Coulomb-dipole theory -- which I did not dwell upon in my most recent articles²⁻⁵ including also the positron-atom impact ionization problem⁶ and two-electron photodetachment of H^- . The latter has particular relevance for this conference in view of the fact that the newest experiment⁸ involves the accelerator (LAMPF) in a basic way.

Outline of Derivation

We are concerned with an electron of energy k_i^2 (in Rydberg units, throughout) impinging on a neutral atom, which we shall take without loss of generality (as we shall see) as hydrogen. In Figure 1, I have outlined the basic mathematical quantities that one must deal with starting with yield of positive residual ions which is (one half) the number of the outgoing electrons integrated over all momenta subject only to the conservation of energy. The expression for $\mathcal{Q}$ is one form of

Basic Quantum Mechanical Expressions

$$\mathcal{Q}(E) = \int \mathfrak{M}^2 d(E - k_1^2 - k_2^2) d^3k_1 d^3k_2$$

where

$\mathcal{Q}(E)$ = yield of positive ions $\vec{k}_i, \vec{k}_1, \vec{k}_2$ = momenta of incident and outgoing electrons

$E = k_1^2 + k_2^2 = k_i^2 - I_{\text{target}}$ = available energy after ionization

$\mathfrak{M} = \langle \Psi_f | V_i | \Phi_i \rangle$ = transition matrix element, in final state form.

$\Rightarrow \Phi_i$ = initial state (unperturbed $\equiv$ sol. of Schröd. eq. in absence of V_i)

Ψ_f = final state (exact sol. of complete Schröd. eq. with appropriate boundary conditions)

Threshold law $\equiv$ functional dependence on E of $\lim_{E \rightarrow 0} \mathcal{Q}(E)$.

Fig. 1 Basic expressions for quantum mechanical theory of the threshold law.

Fermi's Golden Rule of which the chief component is the transition matrix element $\mathfrak{M}$ from an initial to final state. We shall discuss that in the next two slides, but first note that the threshold law is defined as the functional dependence of $\mathcal{Q}$ on E in the limit $E \rightarrow 0$. The fundamental dynamical quantity will be dealt with in a form in which the initial state is unperturbed whereas the final state is in principle the exact solution. There are good reasons⁵ for preferring that form rather than the initial state form for inferring the correct (mathematical) form of the threshold law.

The interaction V_i is the part of the total potential not represented in Φ_i . In order to simplify the problem we deal not only with one partial (total S) wave, but with a two-dimensional model² whereby the electrons are treated as if they were strictly on opposite sides of the nucleus. Again let me just say that there are strong reasons to believe that these simplifications will not affect the mathematical form of the threshold law.^{2,4,5}

The physical question which underlies the controversy surrounding the threshold law is

pictorially represented in Figure 2; it comes down to what configurations are likely to result from the ionization process. On the top you see that the Wannier theory⁹ assumes that the electrons emerge on essentially opposite sides of the nucleus and with nearly equal momenta. Mathematically that

Fig. 2 Contrasting dominant configurations for Wannier vs. Coulomb-dipole theories.

is a saddle point of the potential curve of the whole system; the Wannier theory⁹ can be described as a very incisive classical perturbation theory of orbits near this quasi-stable ridge. The complementary domain pictured at the bottom represents the Coulomb-dipole region; it provides the basis of our approach. If this region is correctly described, one should in principle cleanly be able to determine whether it dominates at threshold by comparing (the energy dependence of) the respective matrix elements. Unfortunately with respect to the Wannier region, one does not a priori know the normalization of that part of Ψ_f ; thus those derivations¹⁰ which translate Wannier's classical analysis into (WKB) wave function form must use an additional (quasi-ergodic) hypothesis which Wannier himself introduced⁹ in his otherwise purely classical analysis to derive his famous threshold law:

$$I_{\text{Wannier}} \propto E^{1.127}$$

The Coulomb-dipole derivation does not require any additional normalization hypothesis: it is sketched in the next figures (3 and 4). In Figure 3, when the inner of the escaping electrons is closer to the nucleus than it is to the outer electron ($r_1 \geq 2r_2$), then it is reasonable to say that the outer electron sees the dipole formed

by the inner electron and the nucleus. (We can substitute residual ion for nucleus for neutral atoms other than H and nothing changes. That is why

Fig. 3 Aspects of Coulomb-dipole final state.

the threshold law has the same form for all neutral targets.) Because $r_1 \geq 2r_2$, it is also consistent to say the inner electron sees only the Coulomb field of the nucleus in the first approximation.

The total wave function $\Psi_f^{(cd)}$ is therefore the product given in Figure 3. But the dipole moment of the instantaneous dipole seen by the outer electron is clearly a function of, in fact equal to, the distance of the inner electron from the nucleus (r_2). But by putting that into the (imaginary) order of the Bessel function describing the outer electron, one is dealing, mathematically, with a highly non-separable function of r_1 and r_2 !

Derivation of (Coulomb-Dipole) Threshold Law [Phys. Rev. Lett. 49, 365 (1982)]

1. Substitute $\Psi_f^{(cd)}$ and Φ_i into $\mathcal{M} = \int d\mathbf{r}_1 d\mathbf{r}_2 \int d\mathbf{r}_3 \Psi_f^{(cd)} \Psi_i^* V \Phi_i$, and obtain

$$\lim_{k_1, k_2 \rightarrow 0} \mathcal{M} = \frac{1}{\sqrt{k_1 k_2}} \left[\frac{\sin(R^2 \ln k_1 + \text{const.})}{R^2 \ln k_1} + 0 \left(\frac{1}{(\ln k_1)^2} \right) \right]$$

2. Substitute $\mathcal{M}$ into $\mathcal{Q} = \int \mathcal{M}^2 \delta(E - k_1^2 - k_2^2) d^3 k_1 d^3 k_2$, and obtain

$$\lim_{E \rightarrow 0} \mathcal{Q}(E) = \frac{E}{(\ln E)^2} \left\{ 1 + \frac{1}{\alpha(R)} \sin[\alpha(R) \ln E + \text{const.}] \right\}$$

where $\alpha(R) \approx R^{1/2}$

Estimate of $R^{1/2}$: find $(r_2) \equiv R$ beyond which $\Psi_f^{(cd)}$ is accurate sol. of Schröd. eq.: $|(H - E) \Psi_f^{(cd)}| / |\Psi_f^{(cd)}| \ll 1$. Find $7 \leq R^{1/2} \leq 160$

Fig. 4 Precis of derivation of threshold law.

In spite of that it turns out that the analytical dependence on energy of the matrix element $\mathcal{M}$ can be deduced to lowest order; and that defines the

threshold law, summarized in the next figure (4). In Fig. 3 note first that the parameter R is pictured as the distance from the nucleus at which the inner electron's path becomes a straight line. For $r_2 < R$, where the classical path is curving rapidly, remembering that quantum mechanical particles are really charge clouds, we might expect that the inner electron shields the nucleus even more effectively than a classical description would suggest. This then is the origin of the lower limit on the integral in Figure 4. More details of the analytic evaluation are given in Ref. 2, but the net result is the threshold law given in the middle of the figure. The result is of interest from many points of view: mathematically not only is $\mathcal{Q}$ not a pure power law in E , but by virtue of the factors multiplying E , it is doubly non-analytic (in the complex variable sense) as a function of E . Nevertheless, both $\mathcal{Q}(E)$ and its first derivative are zero at threshold, and the modulating factor whose sinusoidal part oscillates infinitely rapidly as $E \rightarrow 0$ will not prevent $\mathcal{Q}(E)$ from increasing monotonically (and one can argue cogently that that must be so²) providing $[\alpha(R)]^{-1}$ is small enough; it is gratifying that the estimate of R described at the bottom of Figure 4 does indicate that, and that the experimental fit¹¹ yields such a magnitude as well as (approximately) the reciprocal relation between it and the coefficient found to multiply the $\ln E$ term inside the sine.

Let us come quickly to the experimental attempts to ascertain the threshold law. The most significant and recent experiment of Donahue *et al.*¹¹ (Fig. 5) utilizes the LAMPF accelerator to achieve a high energy beam of H^- ions.

**Experimental Observation of Threshold
by 2-Electron Photodetachment**
J.B. Donahue, Gram, Hynes, Hamm, Frost, H.C. Bryant,
Butterfield, Clark, W.W. Smith, Phys. Rev. Lett. 48, 1538 (1982)

Fig. 5 Two-electron photodetachment experiment (LAMPF) and results.

With such a beam, one can utilize a conventional optical laser and still achieve sufficient relative energy to initiate photo-double detachment of the (H^-) negative ion. The most significant advantage of a photon experiment is that one can and does achieve much finer energy resolution (0.007 eV) of the beam, than can be obtained with an electron beam. And the experimental results, seen at the bottom of the figure, confirm that. They are fit (solid curves) by our prior² linear modulated law as well by the Wannier threshold law. One sees that the fits are comparable; although the respective solid curves look quite different from each other very close to threshold. In fact the confidence level, which is roughly proportional to the inverse of the root mean square error times the number of adjustable parameters in the mathematical form being tested, is somewhat better for our modulated linear law. To fit data to our present form of $\mathcal{Q}$, the E factor in $(\ln E)^{-2}$ should most naturally be scaled by ER^2 , where R (Fig. 4) defines the Coulomb-dipole region i.e., $(\ln E)^{-2} \rightarrow [(\ln (ER^2))]^{-2}$. The threshold region should therefore be confined to $E < R^{-2}$; from our estimate of R this implies not more than 5 meV above threshold. If one nevertheless fits our form for $E > R^{-2}$, then as long as $|\ln E| \ll |\ln R^2|$ the form reduces effectively to a modulated linear law. This is our interpretation of the present experimental fit.¹¹ Thus with regard to that experiment, its present significance is that for the first time another form (other than linear and $E^{3/2}$) has now been tested against the Wannier law and shown that it can be just as successful. Prior work (cf. particularly Ref. 12) was untested in this regard. This circumstance, among other things, demonstrates the truism that one can never prove a threshold law experimentally!

Returning to the experiment of Donahue *et al.*¹¹, there are intrinsic errors that cannot completely be avoided. The most important practical effect is due to field ionization caused by the deflecting magnetic field used to separate off the H^+ ions; that deflecting magnetic field, which is seen as an electric field by the rapidly moving hydrogen beam, can field ionize highly excited hydrogen atoms which can also be formed by the laser:

motional electric field + $H(N) \rightarrow H^+ + e_2$.

The latter reaction will cause a spurious yield of H^+ ions. The LAMPF experiment¹¹ has successfully reduced the minimum $N \geq 15$, and concluded that the only effect is to reduce the apparent threshold by 0.05 eV to 14.305 eV.

Even if one were able to get rid of the motional field effect altogether (for example, say one could do the experiment with conventional lasers and stationary negative ions -- which in fact is being attempted) there would still be a residual background effect whereby blackbody photons corresponding to (room temperature) heat can provide the second step in achieving two-step photo-double detachment:

$(h\nu)_{\text{blackbody}} + H(N) \rightarrow H^+ + e_2$.

Blackbody Correction [A.T. Phys. Rev. A22, 324 (1980)]

Two-electron photodetachment can be contaminated by 2-step process

Probability of (II) described by

$$P_N(T) = \frac{1}{2} \int_0^\pi d\theta \left\{ \int_{\omega_{\text{res}}} \sigma_N(\omega') I_T^{(\text{Planck})}(\omega) d\omega \right\} \quad \text{where} \quad \begin{cases} \sigma_N(\omega') = \frac{64}{3} \frac{\alpha \pi}{(\omega')^3} \frac{1}{N^3} \\ \omega' = \gamma \omega (1 - \beta \cos \theta) \\ \beta = \frac{v_H}{C} \quad \gamma = (1 - \beta^2)^{-1/2} \end{cases} \quad \text{Seaton, (1959)}$$

$$\text{Since } \sum_N^{N+AN} |\mathbf{M}_N|^2 \xrightarrow{\text{analytic continuation}} \int |\mathbf{M}_{N(\omega)}|^2 N^3(\omega) d\omega = \frac{1}{2} \gamma_{2e}(E) \quad \omega = +N^2, E = \omega + k_i^2$$

$$\begin{aligned} \text{then } \gamma_{\text{corr}} &\propto k_B T \sum_{N_{\text{min}}}^{N+AN} |\mathbf{M}_N|^2 \frac{1}{N^3} \propto (k_B T)^{7/2} \frac{(\ln E)^2}{E} \gamma_{v_{2e}} \quad \beta = v_H / c \\ \Rightarrow \gamma_{\text{obs}} &= \gamma_{v_{2e}} [1 + f(\beta) (k_B T)^{7/2} \frac{(\ln E)^2}{E}] = > \left\{ \gamma_{\text{corr}} \leq \frac{1}{10} \gamma_{v_{2e}} \right. \\ &\quad \left. \text{for } E \geq 10^{-3} \text{ eV} \right\} \end{aligned}$$

Fig. 6 Blackbody correction to photo-double detachment.

It turns out⁷ that this effect can be calculated. The analysis is summarized in Figure 6, but in view of the modification of the new threshold law,³ the formula we derived in Ref. 7 must be slightly modified to read as given in γ_{obs} in Figure 6, where $f(\beta)$ is a function of β which can be evaluated.⁷ The original correction⁷ is here modified such that γ_{corr} is finite, as it must be in the limit $E \rightarrow 0$. We now find that the blackbody correction term is negligible only for $E \gtrsim 10^{-3}$ eV, using room temperature and parameters of the LAMPF experiment.¹¹ That is a factor ten larger than our original estimate⁷ based on the modulated linear threshold; and it implies that the blackbody correction is already on the verge of observability!

We conclude this presentation with a very brief exposition of the positron impact ionization threshold. Positron interactions have recently become of importance in space physics. An example in the observation of the positron-electron annihilation γ -ray line from the direction of the galactic center;¹³ the knowledge of low energy positron interaction cross sections has enabled preliminary astrophysical understanding of the source region.¹⁴ Of relevance to this conference, the modern era of low-energy positron experiments was initiated by an accelerator experiment,¹⁵ wherein high energy electrons struck a target and eventually produced electron-positron pairs; the positrons were slowed down in a moderator from which, through the workings of a non-trivial solid state effect, an unusually large flux of almost monoenergetic, low energy positrons emerged.¹⁶ That provided the source of the low energy positron beam used for the scattering experiment.¹⁵

From the point of view of theory positron interactions with atomic systems provide an interesting and non-trivial contrast to electron scattering. This applies to the impact ionization threshold as well.

Positron (vs. Electron) Impact Ionization Threshold

Not only is $\lim_{E \rightarrow 0} \gamma_{\text{Klar}}^{(+)} < \gamma_{\text{cd}}^{(+)}$ but $\gamma_{\text{Klar}}^{(+)} < \gamma_{\text{phase space}} = \int d^3k_1 d^3k_2 d(E - k_1^2 - k_2^2)$
Question: validity of the quasi-ergodic hypothesis?

Fig. 7 Aspects of the e^+ -atom (vs. e^- -atom) threshold.

In Figure 7 you see in a very pictorial way that corresponding to the two final state configurations for threshold electron impact ionization that we have discussed above, there are two regions for positron impact ionization: Coulomb-dipole and continuum positronium formation mechanisms. The differences from the respective electron configurations are the result of the attraction rather than repulsion between the two outgoing leptons. In particular the "formation of

positronium in the continuum" is the clear analogue of "charge exchange into the continuum," which is now well established in heavy particle ion-atom impact ionization.¹⁷ We have argued that the positron threshold is determined by the Coulomb-dipole mechanism and will give rise to the same form of threshold law,⁶ because again the slow electron is much closer to the nucleus than it is to the more distant positron. The only difference from the corresponding electron impact case is that the electron emerges on the same side as the positron, but other than that the angular dependence (on $\hat{r}_1 \cdot \hat{r}_2$) is expected also to be weak.⁶ In contrast, continuum positronium formation is the geometrical inverse of the Wannier mechanism, and I believe the threshold law for it corresponds to the one recently worked out by Klar.¹⁸ As seen in Fig. 7 the result, $\mathcal{Q}_K \propto E^{2.65}$, is not only different from and much smaller than all others, but even smaller than phase space, which can be shown to be proportional to E^2 . Physically I believe the high power of E in Klar's result derives from the sensitivity to the angle of the positron electron line relative to the direction to the center of mass:⁶ only when $\theta \approx 0$ is it probable that the positronium in a continuum state will emerge near threshold.

Physically however, it is very difficult to believe that a process will be dominated by such an unlikely mechanism, when another mechanism is readily available. What then is wrong with these essentially classical derivations? I have discussed that in Ref. 5: I believe the weak point is Wannier's quasi-ergodic hypothesis⁹ which is also invoked by Klar.¹⁸ It is the assumption that the orbits of double escape preserve a geometrical similarity whose energy dependence is inherent in Newton's equations with Coulomb forces, providing the distribution of initial conditions are random on some inner surface outside of which the classical equations are valid. However, I have argued⁵ that if only a minute portion of the wave function corresponds to impact ionization, then it is extremely unlikely this portion will be suitably independent of E even if the wave function as a whole is. The cogency of the purely quantum mechanical approach is that it completely avoids the quasi-ergodic hypothesis. And in the case of positron ionization this hypothesis puts a particularly severe constraint on (Klar's) threshold law, which, when viewed quantum mechanically, is

very unrealistic and which more significantly, may be experimentally testable in the not too far distant future.

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