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The Energy Distribution Cross Section in Threshold
Electron-Atom Impact Ionization

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ABSTRACT

The flatness of the energy differential cross section in impact ionization is derived analytically in the Wannier theory. However it is shown that the Wannier zone is confined to a region of the order $E/5 \leq \epsilon \leq 4E/5$, where E is the available energy and ϵ is the energy of one of the electrons. By contrasting the known results of photoionization and photodetachment, one can cogently argue that in the complementary region where the electrons share their energy very unequally the cross section rises to a value independent of E (aside from a modulation factor) and that this region determines the form of the threshold law.

The recent measurements of Cvejancovic and Read (1974) of electron-helium ionization have given renewed impetus, since the classic experiment of McGowan and Clarke (1968), to studies of the electron-impact threshold law, and to the Wannier (1953) theory in particular. The specific aspect of the recent experiment that we wish to discuss is the energy distribution cross section $dQ/d\epsilon$, where ϵ is the energy of one of the electrons (E being the total available energy) and Q is the total yield of positive ions of charge Z . $dQ/d\epsilon$ could be a function of both

E and ϵ , but what the experiment finds is that $dQ/d\epsilon$ is in fact independent of ϵ . (In view of the concluding discussion we emphasize that the experiment does not cover the whole range, and the region of linearity is confined roughly to $1/5 \leq \epsilon/E \leq 4/5$.) This result has never been shown analytically on the basis of the Wannier theory, but has emerged from numerical integration of Newton's equations (Vinkalns and Gailitis, 1967a, b, Banks et al. 1969. Peterkop and Tsukerman 1969, 1970, Grujic, 1972). We shall show first within the confines of the theory that the result can be obtained analytically.

We start with the solutions in the Coulomb zone where the kinetic and potential energies are separately much greater than the total energy, $E \ll Z/r$. In this region the relevant classical solutions leading to double escape are (Vinkalns and Gailitis, 1967a, b)

$$r_{1,2} = r \pm C_2 r^{3/4 + \mu/2} \quad (1)$$

where μ is the Wannier parameter

$$\mu = \frac{1}{2} \sqrt{\frac{100Z - 9}{4Z - 1}}, \quad (2)$$

The double escape occurs with the electrons going in essentially opposite ($\theta_{12} \cong \pi$). In this circumstance the hyperradius and radial difference vector reduce to the scalars

$$r = \frac{r_1 + r_2}{2}, \quad \Delta r = \frac{r_1 - r_2}{2} \quad (3)$$

The solution (1) is only valid if $\Delta r \ll r$, thus it assumes that both electrons are at approximately equal distance from the ion, so that the total potential energy,

$$V = -\frac{1}{r_1} - \frac{1}{r_2} + \frac{z}{|r_1 - r_2|} \Bigg|_{\text{WANNER}} \approx -\frac{2z + \frac{1}{2}}{r}, \quad (4)$$

can be thought of as divided equally between each particle. We evaluate the ratio of individual total energies therefore from

$$\frac{E - \epsilon}{E} = \frac{\frac{1}{2} \dot{r}_1^2 + \frac{1}{2} V}{\frac{1}{2} \dot{r}_2^2 + \frac{1}{2} V}. \quad (5)$$

Using the derivative formulae (Vinkalns & Gailitis 1967)

$$\dot{r}_{1,2} = \left[1 \pm C_2 \left(\frac{3}{4} + \frac{\mu}{2} \right) r^{-1/4 + \mu/2} \right] \left(E + \frac{2z - \frac{1}{2}}{r} \right)^{1/2}$$

together with (1), (2) and (4) in Eq. (5) gives to lowest order, the desired relation

$$C_2 = \frac{E^{\mu/2 - 1/4}}{(3 + 2\mu)} \frac{(\rho z)^{5/4 - \mu/2}}{\left(z - \frac{1}{4} \right)} \left(1 - \frac{2\epsilon}{E} \right) \quad (6)$$

where C_2 has been evaluated at a point $r = \rho Z/E$.

Formula (6) checks very well with numerical solutions (Vinkalns & Gailitis, 1967a, b); it is to be emphasized however that the numerical solutions are obtained by integrating Newton's equations through the Coulomb zone into the free zone. What (6) establishes than in combination with the numerical results is that the energy distribution between the two electrons is unaffected by their passage through the Coulomb zone.

The question of the threshold law then comes down to the distribution of C_2 as the particles enter the Coulomb zone. It is universally agreed that this is a quantum mechanical problem. The Wannier assumption is that the wave function in the interior is very complicated and therefore very insensitive to the exact value of E . Thus the C_2 are randomly distributed (quasi-ergodic hypothesis), in which case the cross sections are given by (Vinkalns & Gailitis 1967)

$$Q \propto C_2^{(\max)} \propto E^{\mu/2 - 1/4} \quad (7)$$

$$\frac{dQ}{d\epsilon} \propto \frac{dC_2}{d\epsilon} \propto E^{\mu/2 - 5/4} = \text{independent of } \epsilon \quad (8)$$

both of which can readily be derived from (6).

Formula (7) is the Wannier threshold law, and (8) is the analytic expression of the flat energy distribution cross section. The correctness of these results therefore depends on the validity of the quasi-ergodic hypothesis. The following

shows that (8) is not valid over a sufficiently large range of ϵ to invalidate the Wannier law for the total cross section (7). It is understood that this argument applies to the quantum zone.

Consider the problem of photoionization (neutral atom target) versus the one of photodetachment (negative ion target). If one were to use a classical analogy, one might expect that photoionization would exhibit a smaller yield at threshold than photodetachment, because the electron and residual ion attract each other much more strongly in the final state and thus have a smaller chance of separating than electron neutral pair in the case of photodetachment. In fact this argument is wrong: photoionization has a finite threshold value in contrast to photodetachment which is zero at threshold. The reason is that quantum mechanically the process should not be considered as evolving slowly in terms of an orbit but rather as occurring instantaneously. The probability of transition then becomes the fundamental mathematical quantity, and that is controlled by the length of time that the emergent particle stays in the vicinity of the residual ion; which in turn is characterized by the $k^{-1/2}$ normalization factor for photoionization as opposed to an energy independent normalization factor in the case of photodetachment. Now consider the problem of double photodetachment (of a negative ion). Although the transition operator is somewhat different, it can confidently be argued that the yield is proportional to the same threshold law that governs electron-atom impact ionization. If one applies the Wannier arguments (Roth

1972), then one derives the same Wannier law, and one additionally argues that if the energies of the two electrons are too dissimilar, then the slower electron will not emerge. In fact, however, the above arguments concerning single photoionization show that it is exceedingly likely that the slow electron will emerge, providing the faster electron can also escape. That the faster electron can also escape is assured by observing that it is described by an equation (Temkin-Hahn 1974)

$$\left[\frac{d^2}{dr^2} + \frac{b(\epsilon)}{r^2} + \frac{\gamma(\epsilon, E)}{r^4} + k_\epsilon^2 \right] u_{k_\epsilon}(r) = 0 \quad (9)$$

where $k_\epsilon^2 = E - \epsilon$.

The $b r^{-2}$ is the dipole potential of the nucleus of inner electron and γr^{-4} is a closure approximation of the remaining part of the optical potential (whose structure strongly suggests the γ is an oscillating function of ϵ, E). The significance of this, because of the presence of the r^{-2} potential, is that it too is governed by a normalization factor $\eta(\epsilon)/k_\epsilon^{1/2}$ (Temkin, Bhatia; and Sullivan 1968). The η factor is modulated, but a bounded function of ϵ , therefore the dominant factor is $k_\epsilon^{-1/2}$ which then similarly enhances the probability of its escape as $k_\epsilon \rightarrow 0$. The net result is that as $k_\epsilon (> \epsilon) \rightarrow 0$ the energy distribution cross section approaches a value independent of k_ϵ and ϵ , hence E (except for a modulation factor).

On the basis of these arguments we can sketch the energy distribution cross section in Fig. 1. There we show for four total energies $E_i < E_{i+1}$ that the

flat middle (Wannier) parts of the curves are diminished according to $E^{\mu/2-5/4}$ ($= E^{0.127}$ for electron-atom ionization or double electron-negative ion photo-detachment) whereas the inner regions ascend to a value independent of E aside from a modulation factor. The size of the region away from the Wannier zone (which is pictured as rising smoothly but could readily contain substructure) may be estimated as corresponding to distances of the inner electron closer to the nucleus than to the radial distance of the outer electron from the nucleus ($r_2 < 1/2 r_1$). As long as we are in the free zone, $r_2/r_1 \propto \dot{r}_2/\dot{r}_1$ and since $\epsilon_1 = 1/2 m \dot{r}_1^2$, then $r_2 < 1/2 r_1$ translates into $\epsilon_2 \ll (1/4) \epsilon_1$, where $\epsilon_2 = k_e^2$ and $\epsilon_1 = \epsilon$. Thus using $\epsilon_1 = E - \epsilon_2$ we obtain

$$\epsilon \leq \frac{1}{5}E, \quad \epsilon \geq \frac{4}{5}E \quad (10)$$

as the regions of enhancement. Although the exact constants in (10) may be uncertain, the essential feature of (10) is the linear dependence on E. For that implies that the total yield is dominated by the wings and is a linear function of E times whatever modulation factor is operative there. In Temkin-Hahn (1974) we have proposed

$$Q \propto E [1 - C \sin(A \ln E + B)] \quad (11)$$

The constants in (11) can be adjusted to be virtually indistinguishable from the Wannier law in the presently experimentally accessible threshold region ($0.04 \text{ eV} < E < 0.1 \text{ eV}$). At lower energies however, (11) will yield a much larger value oscillating about a linear law.

The best way of experimentally probing this low energy region is through double photodetachment of negative ions using the newly emerging laser techniques. Indeed if one can do multiphoton double photodetachment, then one can avoid the large single photon energy requirement and simultaneously probe angular momentum states different from the dipole allowed ones for single photoionization.

CAPTION

Figure 1. Energy distribution curves for four total energy. Each curve is symmetric about its midpoint $\epsilon = 1/2 E_i$. Only the first half of each is pictured.

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