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Doubly Excited States of H^- of High Principal Quantum Number: Implications for Electron-Atom Ionization

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It is pointed out that insight into the threshold region of electron-atom ionization can be gained by examination of the nature of the doubly excited states of the compound ion. A study of these states for H^- has been initiated with two types of variational wave functions. One, Ψ_W, has the two electrons at roughly equal distances from the nucleus; the other, Ψ_D, has one electron at a very much farther distance so that it sees the dipole potential caused by the inner electron and the nucleus. Both functions are constructed to be eigenfunctions of the operator Q_N, which projects out all states of the target of principal quantum number less than N, and renders the energy subject to a minimum principle. If the number of states for which Ψ_W yields a lower energy than Ψ_D is proportional to N^γ, then an extrapolation argument shows that the threshold yield curve will be effectively proportional to $E^{(3-\gamma)/2}$. Calculations have been done to $N=5$ for Ψ_D and $N=9$ for Ψ_W. Only the lowest of the Ψ_W states is lower than the corresponding Ψ_D state. The results suggest γ in the range $0<\gamma\leq\frac{1}{2}$. Some comments on Wannier's theory of ionization are made.

I. INTRODUCTION

The theory of low-energy electron-impact ionization of atoms by electrons is fraught with difficulties from beginning to end. The difficulties are both mathematical and conceptual in nature. The mathematical difficulties derive from the long-range nature of the Coulomb potential combined with the intrinsically three-body nature of the wave function in the final state. In almost all cases, however, these problems are related to conceptual questions of immediate physical significance. If the two electrons come away from the nucleus or residual ion (considered an infinitely heavy point charge and always referred to as the nucleus) with approximately equal and opposite velocities, then it is a reasonable argument that each electron sees the nucleus directly and that classical mechanics can be applied.[1] The point here, of course, is the virtual identity of Coulomb scattering in classical and quantum mechanics and the fact that the classical approximation becomes more exact as the energy gets lower. If, on the other hand, the electrons come off with quite different velocities, the validity of classical mechanics is a much more questionable item. Here the quantum mechanical argument is that the inner electron may shield the outer electron from the nucleus thereby making the potential it sees shorter range than Coulombic. In that case its behavior may not be governed by classical mechanics, and the classical approximation may get poorer as the energy is lowered.[2] The classical or classical-like arguments have the general effect of leading to near linear[1] or linear[3] threshold law. Specifically the latter has been deduced by taking an asymptotic form that has been derived for the wave function describing the two outgoing electrons[4] as being essentially two-Coulombic in nature. On the other hand, the shielding argument leads to an $E^{3/2}$ threshold law because only the inner electron is Coulombic. The disparity of these results has naturally promoted a controversy as to which if any of these threshold laws is correct.

It is the purpose of this paper to examine some of these questions from a consistently quantum mechanical point of view. We shall attempt to avoid questions concerned with the controversial[2] asymptotic form above threshold[3,4] by considering the process as a continuation of real or virtual processes below threshold. It also allows calculations to be done in a fairly unambiguous way. We believe that this is the most important aspect of our work, for if any question be raised concerning the variational forms of our wave functions, the way has been opened for other forms to be proposed and tested on the impartial balance of quantitative comparison. The one question that this approach can probably not answer is any subtle questions of analytic continuation from negative to positive energies. We shall be more detailed concerning what effects we believe this can have in Sec. III; for the present it is only relevant to note that the one advantage of the two-body Coulomb force is that the continuum solution merge continuously with the discrete solutions. Similarly, if we correctly describe the major physical situations that can occur below threshold in the three-body problem, then we can reasonably suppose that what we extrapolate them to be will be substantially correct.

What are the physical processes which extrapolate to ionization? They are of two types: (1) Inelastic processes in which the orbital electron is raised to a highly excited state N with N finally going into continuum, and (2) double excitations in which both particles can be considered simultaneously caught in an excited "bound" state, also it will turn out, characterized by the principal quantum number N, where again N finally goes into the continuum. Whereas the former are real both in the sense that they occur at energies above the energy necessary to excite the Nth level and the processes correspond to rigorous time-independent solutions of the Schrödinger equation, the double-excitation processes can be considered virtual inasmuch as they occur below threshold and they do not correspond to rigorous time-independent solutions of the Schrödinger equation.[5] Nevertheless they do occur, and they can have a profound effect on the scattering both below and above the thresholds in question.

The threshold law is derived by summing all inelastic cross sections in the neighborhood of an excited state N and analytically extrapolating the result in N to positive-energy states. The relevant matrix element is the transition amplitude for scattering from the ground to the Nth state. But the key point is that the secular dependence of this matrix element on N is not determined by the inelastic wave function in its asymptotic region but in a more interior region. Just where this interior region is and what the relevant form of the wave function is there is monitored by the doubly excited states. The point here is that the inelastic wave function at threshold is dominated by its resonant behavior below threshold.

In Sec. II we deal with doubly excited-state calculations and in Sec. III with the derivation of the threshold law. One of the forms of the doubly excited wave function has been motivated by Wannier's theory of ionization[1] according to which the threshold law is dominated by processes in which the energies and the radial distance of the escaping electrons are not too different from each other. In Sec. IV we discuss his theory a little more and point out that his derivation cannot be justified in a completely classical theory of electron-atom (or ion) ionization.

The second form of wave function is one wherein the outer electron naturally sees an r^{-2} potential coming from the degenerate perturbation of the states describing the inner electron. This potential causes a change in the normalization factor when this function is extrapolated into a continuum inelastically scattered function which in one respect makes it appear like a Coulomb function. This derivation is the subject of the Appendix, but it is also shown there that notwithstanding the normalization factor, the ionization threshold law coming from such states is essentially the same as that given by the Born approximation ($E^{3/2}$). Here it should be emphasized that although the calculations are done for the e-H system, that the results should hold for electron-atom systems generally because atomic states become hydrogenic for large N.

II. DOUBLY EXCITED STATES OF H$^-$

We shall calculate doubly excited (i.e., autoionization) states of H$^-$. There are two reasons for dealing with this negative ion: first it is the simplest negative ion, but more important the eigenfunctions of the target atom are known exactly and therefore we can use the Q-operator technique[6,7] without approximation. Also following Wannier[1] we shall deal with only total S states in the belief that the threshold law cannot be altered in form by higher angular momentum states.

The two wave functions which we use are[8]

$$\Psi_W^{(N)} = \sum_{l=0}^{N-1} C_{\nu Nl} \frac{R_{\nu l}(r_1)}{r_1} \frac{R_{Nl}(r_2)}{r_2} \times P_l(\cos\theta_{12}), \quad \nu \geq N \tag{2.1}$$

and

$$\Psi_D^{(Nj)} = \frac{v_{Nj}(r_1)}{r_1} \sum_{l=0}^{N-1} B_{lj}^{(N)} \frac{R_{Nl}(r_2)}{r_2} \times (-1)^l (2l+1)^{\frac{1}{2}} P_l(\cos\theta_{12}). \tag{2.2}$$

The physical meaning of $\Psi_W^{(N)}$ is easily understood; it describes the two electrons in doubly excited states at roughly equal radial distances from the nucleus. (We assume $\nu \cong N$.) The functions $R_{Nl}(r)$ are r times the radial-hydrogen wave function. The angular correlations indicated by the electron-electron repulsion are taken up by the linear variational parameters $C_{\nu Nl}$ of which $N-1$ are effectively free and one is determined by normalization. Physically it is clear that the calculation will make them such as to concentrate the electrons on opposite sides of the nucleus. It is also clear that for neither particle does this function contain states of hydrogen with principal quantum less than N. I.e., for $i=1, 2$,

$$\int R_{n\lambda}(r_i) Y_{\lambda m}(\Omega_i) \Psi_W^{(N)} d^3 r_i = 0, \quad n<N, \quad \lambda<n. \tag{2.3}$$

Thus the function is an eigenfunction of the Q_N operator,[9] and variational calculations will give eigenvalues which, if they lie below the Nth state of the hydrogen atom, will correspond to resonances in the elastic and inelastic channels.

Although the physics of $\Psi_D^{(Nj)}$ is also readily understood, the mathematics needs some explanation. The following is a precis of Mittleman's[10] generalization to arbitrary N of the analysis which Temkin and Walker[11] have given for the $N=2$ state. Let us start with the following ansatz for the closed-channel wave function:

$$\Psi_D^{(N)} = \sum_{l=0}^{N-1} \frac{u_{Nl}(r_1)}{r_1} \frac{R_{Nl}(r_2)}{r_2} \times (-1)^l (2l+1)^{\frac{1}{2}} P_l(\cos\theta_{12}). \tag{2.4}$$

The functions $u_{Nl}(r)$ are to begin with undetermined functions. [The factor $(-1)^l(2l+1)^{1/2}$ is the essential part of the Clebsch-Gordan coefficient by which $Y_{lm}(\Omega_1)$ and $Y_{l-m}(\Omega_2)$ couple to form $P_l(\cos\theta_{12})$.] If one varies the u_{Nl} in the expression for expectation of the energy, then one arrives at coupled differential equations whose longest range terms are of the order r^{-2} and to that order the equations may be written

$$\left(\frac{d^2}{dr^2} - \frac{\mathcal{B}^{(N)}}{r^2} - \epsilon\right) U^{(N)} = 0. \tag{2.5}$$

$U^{(N)}$ is a column vector of the u_{Nl} and $\mathcal{B}^{(N)}$ is a tridiagonal symmetric matrix whose elements are given by

$$\mathcal{B}_{ll'}{}^{(N)} = [l(l+1)/r^2]\,\delta_{ll'}$$
$$+ 3Nl'[(N^2 - l'^2)/(4l'^2 - 1)]^{\frac{1}{2}}\,\delta_{l+1,\,l'}$$
$$+ 3Nl[(N^2 - l^2/4l^2 - 1)]^{\frac{1}{2}}\,\delta_{l,\,l'+1}\,. \qquad (2.6)$$

Introducing the transformation

$$V^{(N)} = B^{(N)}U^{(N)} \qquad (2.7)$$

such that $B^{(N)-1}\mathcal{B}^{(N)}B^{(N)}$ is diagonal, we find that the components of the column vector $V^{(N)}$ satisfy the equation

$$\left(\frac{d^2}{dr^2} - \frac{b_{Nj}}{r^2} + \epsilon_{Nj}\right)v_{Nj}(r) = 0, \quad j = 1,\ 2,\ \ldots,\ N, \qquad (2.8)$$

where b_{Nj} are the eigenvalues of $\mathcal{B}^{(N)}$. Let $B_{lj}{}^{(N)}$ be the associated eigenvectors, then the function $\Psi_D{}^{(N)}$ of Eq. (2.4) takes on the form of Eq. (2.2) and acquires an additional "quantum" number j which orders the sequence of eigenvalues of $\mathcal{B}^{(N)}$ and their corresponding eigenvectors.

Of the N eigenvalues, b_{Nj}, a certain number, $j = 1,\ 2,\ \ldots,\ J_D$, will be negative, and for those functions the equations will asymptotically contain an attractive r^{-2} potential. For each N and j the corresponding equation will contain an infinite number of negative eigenvalues which to an excellent approximation are related by[11]

$$|\epsilon_{Nj}{}^{(s+1)}| = e^{2\pi/\alpha_{Nj}}|\epsilon_{Nj}{}^{(s)}|; \quad s = 1,\ 2, \ldots\ , \qquad (2.9)$$

where $\alpha_{Nj} = (|b_{Nj}| - \tfrac{1}{4})^{1/2}$. (2.10)

The solutions of those equations are Hankel functions[11,12]

$$H_{i\alpha_{Nj}}(i|\epsilon_{Nj}|^{1/2}r)$$

which asymptotically approach $\exp(-|\epsilon_{Nj}|^{1/2}r)$. At short distances Eq. (2.8) becomes altered and essentially nonlocal in character. In fact the attractive r^{-2} potential must become less singular, for the r^{-2} solutions are not regularly behaved at the origin.

For variational purposes we have taken

$$v_{Nj}(r) = e^{-ar}\sum_{m=1}^{q} C_m r^m. \qquad (2.11)$$

In order that $\Psi_D{}^{(Nj)}$ be an eigenfunction of Q_N, it is necessary that

$$\int_0^\infty v_{Nj}(r)R_{n\lambda}(r)dr = 0, \quad n < N, \quad \lambda < n. \qquad (2.12)$$

Note that the Q_N operator is symmetric.[7] Although the form of $\Psi_D(Nj)$, Eq. (2.2), appears to contain no bound states of lower N for the target particle ($\vec{r}_2$), it might contain lower states in the exchanged coordinate ($\vec{r}_1$). In order that the calculation be subject to a minimum principle and in a one-to-one correspondence with resonances, the possibilities of ordinary exchange inelastic scattering from a state lower than N must also be excluded. Equations (2.12) guarantee this to be the case. For a given N there are a total of $q - 1$ values of n and λ for which (2.12) must be satisfied, where

$$q = 1 + N(N-1)/2. \qquad (2.13)$$

If the $v_{Nj}(r)$ contains exactly q terms, then together with normalization all the coefficients are unique functions of a. Thus for variational purposes the function $\Psi_D{}^{(Nj)}$ contains only one variational parameter, a, as opposed to $\Psi_W{}^{(N)}$ which, as was stated, contains $N-1$ parameters. It is very important to realize, because the W and D calculations are based on the same Q_N operator, that the shifts Δ_Q are ideally the same and therefore can be omitted in the comparison of the respective energies that will be made (Table III).

The matrices $\mathcal{B}^{(N)}$ were inverted for all $N = 2$ to $N = 100$. The number of negative eigenvalues is clearly linear with N as is evident from Fig. 1 in which J_D is plotted as a function of N. In fact it is quite certain that

$$J_D = \tfrac{1}{2}N - (\text{lower order in } N), \qquad (2.14)$$

where the term in parentheses may very well be a fractional power of N. The eigenvalues themselves go up quadratically with N. Selected values are given in Table I. The differences in b_{Nj} are seen to be proportional to N and independent of j for the lower values. In fact the b_{Nj} can be fitted to a reasonable approximation by a formula of the form

$$b_{Nj} \cong 3N^2 - B(j)N + C(j). \qquad (2.15)$$

Some feel for the eigenvectors $B_{lj}{}^{(N)}$ can be gleaned from Table II. There it can be seen that aside from a normalization constant $N^{1/2}$ the eigenvectors are fairly independent of j for small l and that they get extremely small for large l as long as j is small. For large j they tend to oscillate and they are of the same order of magnitude.

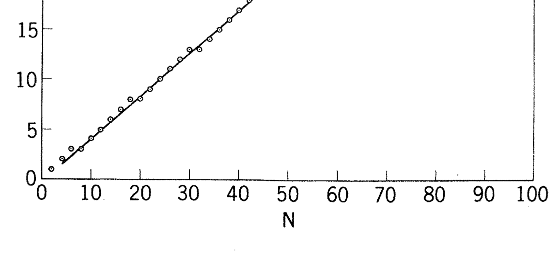

FIG. 1. The number of negative eigenvalues (J_D) vs N. Both J_D and N are defined only on the integers.

TABLE I. Values of $-b_{Nj}$ for selected values of N.

$N(J_D)$ j	10(4)	20(8)	30(13)	40(17)	50(21)
1	262	1123	2584	4646	7307
2	187	971	2355	4339	6922
3	116	822	2128	4035	6541
4	47.4	676	1905	3733	6162
5		533	1684	3435	5786
6		393	1466	3140	5413
7		256	1251	2847	5043
8		122	1039	2558	4676
9			831	2271	4312
10			625	1988	3951
11			423	1708	3593
12			225	1431	3238
13			29.3	1157	2886
14				886.3	2538
15				619.0	2192
16				355.2	1850
17				9.472	1511
18					1175
19					842.7
20					513.7
21					188.2

TABLE III. Comparison of energies (in Ry). Energies are measured relative to the Nth threshold energy $(-N^{-2})$.

N	J_D	a	E_D	$E_W(\nu=N)$	J_W
2	1	0.2	-0.01579[a]	-0.00407	0
3	1	0.2	-0.00992	-0.01272	1
4	2	0.19	-0.00409	-0.00996	1
		0.09	-0.00012	>0	
5	2	0.17	-0.0025	-0.0074	1
		0.11	-0.0005	>0	
6	3	...	...	-0.0056	1[b]
		...	...	-0.00030	
		...	...	>0	
7	3	...	...	-0.0043	$\leqslant 2$[c]
		...	...	-0.00017	
		...	...	>0	
8	3	...	...	-0.00345	$\leqslant 2$[c]
		...	...	-0.0014	
		...	...	>0	
9	4	...	...	-0.00291	$\leqslant 2$[c]
		...	...	-0.0014	
		...	...	>0	
		...	...	>0	

[a] With symmetrization this value reduces to $E_D = -0.375$ at $a=0.25$.

[b] This number is inferred by extrapolation from the values of E_D.

[c] These numbers are upper bounds and are not expected to be the true J_W for all three $N=7, 8, 9$.

The significance of these properties will emerge in the next sections in which we utilize these properties to derive an effective threshold law. We shall also discuss there the significance of the results of the variational calculations. The results themselves are summarized in Table III. The column marked J_W is the number of eigenvalues of the W calculation which are lower than the corresponding eigenvalues of the D calculation. From the foregoing as well as the succeeding discussion this emerges as a very important function of N. It can be seen that we have only calculated it up to $N=5$, although the extrapolation to $N=6$ appears to be quite secure. Note also that J_W is limited to the number of negative eigenvalues of the W calculation. For $N=7$ to 9 this upper bound is two and is also given in the table.

III. IMPLICATIONS FOR THRESHOLD IONIZATION

It may appear that the variational wave functions we have used, in particular Ψ_W, are overly restrictive and that specifically if we had used shielded Coulomb radial wave functions we would have found

TABLE II. A comparison of the eigenvectors $N^{\frac{1}{2}}B_{lj}^{(N)}$ for $N=50$ and $N=100$ and for selected values of l and j.

N	100	50	100	50	100	50	100	50
j \ l	0		1		2		3	
1	0.8027	0.8020	-1.372	-1.354	1.726	1.659	-1.965	-1.817
2	0.8012	0.7990	-1.334	-1.278	1.589	1.392	-1.655	-1.239
3	0.7998	0.7961	-1.296	-1.203	1.455	1.143	-1.367	-0.745
4	0.7983	0.7930	-1.259	-1.129	1.326	0.911	-1.100	-0.329
5	0.7968	0.7900	-1.221	-1.056	1.202	0.696	-0.855	$+0.015$
10	0.7877	0.7741	-1.002	-0.706	-0.544	-0.144	$+0.233$	0.871
20	0.7716	0.7385	-0.656	-0.088	-0.239	-0.815	0.900	0.201
l	4		10		50			
1	2.116	1.857	-1.806	0.880	3.60×10^{-9}	3.75×10^{-16}		
2	1.562	0.877	-0.780	-1.656	1.44×10^{-7}	-2.20×10^{-14}		
3	1.076	0.144	-1.520	-0.520	2.76×10^{-6}	6.35×10^{-13}		
4	0.655	-0.378	-1.281	0.765	-3.37×10^{-5}	-1.20×10^{-11}		
5	0.292	-0.724	-0.630	1.167	2.93×10^{-4}	1.65×10^{-10}		
10	-0.887	-0.770	$+0.819$	-0.911	7.89×10^{-1}	-4.09×10^{-6}		
20	-0.637	0.793	-0.609	-0.602	-0.840×10^{0}	-2.40×10^{-1}		

TABLE IV. The effect on $(E_W)_{N\nu}$ of varying ν in Ψ_W.

N	ν	Lowest root	Second root
8	8	-0.00345	-0.00141
	9	-0.00167	>0
	10	-0.00046	>0
	11	$+0.00015$	>0
9	9	-0.00291	-0.00141
	10	-0.00292	-0.00014
	11	-0.00098	>0

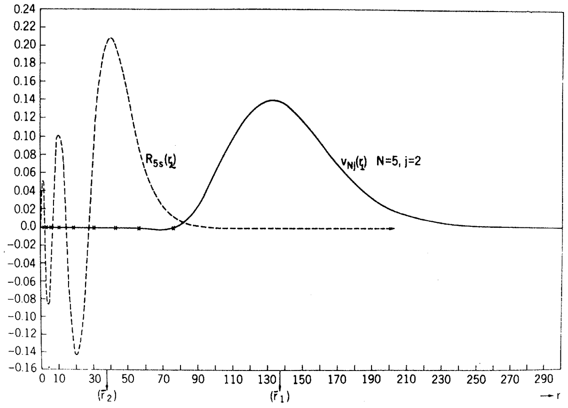

FIG. 2. Comparison of hydrogenic $5s$ function (R_{5s}) and dipole radial function (v_{52}). The fact that the energy of Ψ_D is lower than Ψ_W for the case given indicates that the radial distribution of the two electrons is more accurately given if each is as shown rather than if both were described by hydrogenic functions. The × are the positions of nodes of v_{52}.

more energies of the two-Coulomb type (E_W) lower than their dipole (E_D) counterparts. We do not believe this to be the case for the following reasons. The number of variational parameters in Ψ_W goes up as N, therefore one has more freedom to simulate the effects of shielding, should this have been required. To test this point even further we have varied ν in Ψ_W away from N. The effect of this change can be described as making the mean radial distances of the electrons be slightly different from each other and, thus, to give partial shielding more room in which to operate. The results are summarized in Table IV. It can be seen that in only one case does it reduce an eigenvalue ($\nu = 10$, $N = 9$) and there only the lowest one (which was lower than E_D anyway). Its effect on all higher eigenvalues is to raise them, and in fact in only one case does the second eigenvalue remain bound.

Furthermore, it must be added that the function Ψ_W (for $\nu = N$) is explicitly symmetric whereas Ψ_D is not. Although we do not expect this to be a significant factor for large N, Table III shows that it can have a significant lowering effect for small N. Finally we reiterate that Ψ_D only depends on *one* variational parameter. Thus to the extent that this calculation is biased, it predominantly favors the two Coulomb functions Ψ_W.

Therefore it is the calculations themselves which convincingly demonstrate that the Ψ_D functions dominate. In other words, in most doubly excited states the electrons tend to be at greatly dissimilar distances from the nucleus. For example, in Fig. 2 we see that the second auto-ionization state of the $N = 5$ calculation has a mean radius of r_2 at approximately $37a_0$ whereas $\bar{r}_1 \cong 136a_0$. This in turn can be described as the direct effect of shielding of the outer electron from the nucleus by the inner electron.[2]

However, as will be shown below, the threshold law for ionization will be determined by those few states in which the electrons emerge at comparable distances from the nucleus. The present calculation clearly shows that such equal energy events can occur. In order to extrapolate a threshold law from the present results we shall proceed as follows.[13] To every two-Coulomb auto-ionization state below the Nth threshold, we shall associate an inelastic scattering wave function above the Nth threshold in which the inelastically scattered particle will also be described by a Coulomb wave.

The basis of this association, which is very fundamental to this extrapolation, is essentially that of effective range expansions generally: namely that a continuum function at low energy looks at small distances very much like a bound-state wave function of the same Hamiltonian providing the absolute energy difference of the states is small.[14] For those states which are two-Coulomb-like, the relationship (2.9) will not be accurate between the lowest ($s = 1$) and next lowest ($s = 2$) resonant energies. This is because the interior of the wave function for for $s \geqslant 2$ no longer determines the energy $\epsilon_{Nj}^{(s)}$; however, that is not essential for our purposes. What is essential is that the behavior of the first and second resonant function and all higher resonances as well as the low continuum above the Nth threshold are similar to each other for r_1 and r_2 small, and they are given by Ψ_W.

Similarly to every Ψ_D state which gives a lower energy we shall associate an inelastically scattered wave which asymptotically sees a dipole potential. [In those cases Eq. (2.9) should be accurate for all s.]

Below we shall extrapolate the threshold from Ψ_W states. This can rather cleanly be done and gives the dominant contribution. The contribution from Ψ_D states is considered in the Appendix.

The two-Coulomb wave function above threshold becomes

$$\Psi_D^{(Nj)} \rightarrow \chi_{Nj} = \sum_{l=0}^{N-1} C_{Nlj} \frac{F_l(k_N r_1)}{r_1} \frac{R_{Nl}(r_2)}{r_2} \times P_l(\cos\theta_{12}), \tag{3.1}$$

where $F_l(k_N r_1)$ is a continuum Coulomb function. The index j labels the state of the Ψ_W calculation whose energy is lower than the corresponding j state of the Ψ_D calculation. In general then

$$j = 1,\ 2, \ldots, J_W. \tag{3.2}$$

Although for the results presented in Table III where comparison of D and W calculations can be made, $J_W \leqslant 1$, it must be assumed that as N gets larger, J_W will also. We shall assume that asymptotically for large N, J_W can be represented as

$$\lim_{N\to\infty} J_W \propto N^{\gamma}, \quad 0<\gamma\leq 1. \tag{3.3a}$$

The function χ_{Nj}, however, is an inelastic scattering wave function, and k_N is a wave number of the the inelastically scattered wave. The cross section for excitation of the Nth state is given by

$$\sigma_N = k_N \sum_{j=1}^{J_W} |\langle \chi_{Nj}|V|\Phi_i\rangle|^2, \tag{3.4}$$

where Φ_i is the initial state and V is the interaction

$$\Phi_i = [e^{i\vec{k}\cdot\vec{r}_1}\varphi_0(r_2)]_{S\text{ wave}}$$

$$\propto (\sin kr_1/kr_1)R_{12}(r_2)/r_2, \tag{3.5}$$

$$V = 2/r_1 - 2/r_{12} \tag{3.6}$$

(rydberg units are used throughout). We define the yield to a group of states in the vicinity of the Nth state as Q (not to be confused with the projection operator Q_N):

$$Q = \sum_{N-\Delta N}^{N+\Delta N} \sigma_N\,. \tag{3.7}$$

Now if the energy of the hydrogen atom is labeled $w(N)$, then

$$w(N) = -1/N^2\,, \tag{3.8a}$$

the total energy being given by

$$E = k_N^2 + w\,. \tag{3.8b}$$

When N is large, we can replace the sum in (3.7) by an integral:

$$Q \to \int \sigma_N dN \propto \int \sigma_N N^3 dw\,. \tag{3.9}$$

The matrix element in (3.4) can be written explicitly

$$\langle \chi_{Nj}|V|\Phi_i\rangle \propto \sum_{l=0}^{N-1} \frac{C_{Nlj}}{2l+1}\int_0^\infty\int_0^\infty F_l(k_N r_1)R_{Nl}(r_2)$$

$$\times (r_<^{\,l}/r_>^{\,l+1})\sin(kr_1)R_{1s}(r_2)dr_1dr_2. \tag{3.10a}$$

The normalization factor of R_{Nl} is proportional[15] to $N^{-3/2}$. Since there are N terms in χ_{Nj}, the coefficients C_{Nlj} like the $B_{lj}^{(N)}$, Table II, are proportional to $N^{-1/2}$. (We have verified this to be so up to $N=9$.) The normalization of $F_l(k_N r_1)$ at the origin, corresponding to the Coulomb analog of a plane wave at infinity,[15] is $k_N^{-1/2}$; the sum of integrals over l converges very rapidly[13] and is quite independent of the upper limit. We therefore have

$$\langle \chi_{Nj}|V|\Phi_i\rangle \propto 1/k_N^{1/2}N^2. \tag{3.10b}$$

We shall assume that the dependence on j for N large is secondary, as with the coefficients b_{Nj} of Eq. (2.15), so that the sum over j in (3.4) contributes[16] a factor J_W. Equation (3.9) then leads to

$$Q \propto \int k_N (k_N^{1/2}N^2)^{-2} J_W N^3 dw\,. \tag{3.11}$$

Using (3.3a) for J_W, inverting (3.8a) in the form $N \propto |w|^{-1/2}$, and proceeding into the continuum wherein w is positive and $0\leq w\leq E$ defines the range of integration, we find that

$$Q \propto \int_0^E w^{\frac{1}{2}(1-\gamma)} dw\,. \tag{3.12}$$

Thus finally

$$Q \propto E^{\frac{1}{2}(3-\gamma)}. \tag{3.13a}$$

In order to say something about the value of γ, we have plotted in Fig. 3 the results we have obtained as a function of N. The solid straight line is the same as that in Fig. 1 in the restricted range of N. It represents J_D and therefore is an average of the squares; although it looks somewhat arbitrarily drawn here, Fig. 1 shows that when one goes to larger N there is essentially no ambiguity in it. Similarly the curved lines are intended to represent an average through the open circles (J_W vs N). There are not enough open circles to allow such a curve unambiguously to be drawn; however, as with J_D we expect that going to larger N will allow this curve to be essentially uniquely continued. The limited results do seem to fit better with the smaller fractional value of γ. Further discussion is reserved for the next section.

IV. DISCUSSION

Let us examine some of the assumptions that have gone into the derivation of Eqs. (3.13a). Aside from the material discussed above Eq. (3.1) and the analytic continuation into the positive energy domain, the biggest assumption concerns the summation over j in (3.4). We have indicated[16] that the only error this could reasonably cause is an increase in the exponent in (3.13a). To that extent the exponent $\frac{1}{2}(3-\gamma)$ may be a lower bound on the exponent, which would be quite satisfactory for our purposes. [We believe, however, that it is more accurate than that.] The

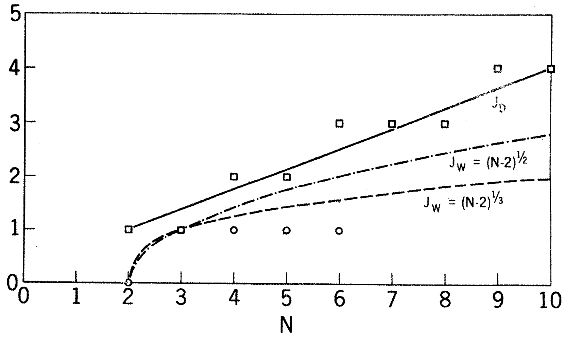

FIG. 3. Solid straight line is J_D vs N representing the squares. The other curves are various analytic fits of the open circles to represent J_W. The constant of proportionality has been chosen to be unity.

process of analytic continuation which is used in going from (3.11) to (3.12) together with the restricted analytic form used to represent $J_W(N)$ may have lost more subtle energy-dependent factors such as $\log E$ or oscillating factors. From most practical points of view logarithmic terms are not important, since they are completely dwarfed by the power-dependent factors; if the factors are oscillating, then we would expect (3.13) to describe the envelope of the curve.

The smallness of J_W in the present calculation might be interpreted to mean either that γ is small or that the constant of proportionality is small in (3.3a). We believe that it is the former which is more suggested by our results; for otherwise one would not have expected $J_W(N)$ to be 1 at $N=3$ and then to remain there to at least $N=7$. Rather one would have expected J_W only to become 1 at a larger value of N. It is for this reason that the agreement of J_W with a fractional power dependence in Fig. 3 appears to fit the limited results so naturally. Note also from Table III that J_W cannot exceed 2 for $N \leq 9$.

Nevertheless it will clearly require much larger N in order for a precise value of γ to be determined. Although we are in the process of extending this calculation, we cannot promise that results will be forthcoming soon. It will require considerably more numerical sophistication to avoid overflow and cancellation of significant figures. (The computer is an IBM 360-91 with approximately 15 significant figure accuracy.)

On the basis of Fig. 3 we would estimate $0 < \gamma \leq \frac{1}{2}$. Indeed the most likely alternate possibility in our opinion would be a logarithmic increase of J_W with N,

$$J_W \propto \log N. \qquad (3.3\text{b})$$

This would change the form of the threshold law to

$$Q \propto -E^{3/2} \log E. \qquad (3.13\text{b})$$

Although we think Wannier's exponent is not correct, our results are not extensive enough to rule it out. (This would correspond to $\gamma \cong 0.75$. Also we cannot rule out a linear theory,[4] $\gamma = 1$, although that seems even more improbable in our opinion.) Wannier's theory, which has recently been revived by Vinkalns and Gailitis,[17] is based on a rather brilliant analysis of the classical orbits (i.e., solutions of Newton's equations) which describe two electrons emerging from the vicinity of the nucleus and not being caught again. Basically Wannier finds for E zero or slightly greater than zero that the solutions are of two kinds:

$$\Delta r = C_1 r^{\frac{3}{4} - \frac{1}{2}\mu}, \qquad (4.1\text{a})$$

$$\Delta r = C_2 r^{\frac{3}{4} + \frac{1}{2}\mu}, \qquad (4.1\text{b})$$

where Δr is the difference of the radial distances of the two electrons from the nucleus (assumed fixed and of charge Z) and r is the mean radius:

$$r = (r_1^2 + r_2^2)^{1/2}, \qquad (4.2\text{a})$$

$$\Delta r = \tfrac{1}{2}(r_1 - r_2), \qquad (4.2\text{b})$$

and $\mu = \frac{1}{2}[(100Z - 9)/(4Z - 1)]$. (4.3)

The first type of solution (4.1a) can exist even at $E=0$, and it corresponds to particles appearing at infinity with equal (necessarily zero for $E=0$) speeds. Geometrically similar solutions continue to exist for $E > 0$, thus the threshold dependence (increase in the number of solutions) is determined by the increase with E of solutions of the second kind (4.1b). These correspond to events in which the two electrons come off with slightly different energies. Wannier[1] has shown that the contribution of these to Q is proportional to C_2 itself. To get the dependence of C_2 on E Wannier appeals to a similarity principle, whereby if

$$\vec{r}_i = \vec{r}_i(t), \quad i = 1,2 \qquad (4.4\text{a})$$

is a solution of Newton's equations for energy E, then

$$\vec{r}_i{}' = B^{-1}\vec{r}_i(B^{3/2}t) \qquad (4.4\text{b})$$

are (geometrically similar) solutions for energy $E' = BE$. The solutions (4.1b) can be written as an explicit function of time using the solution of joint motion

$$r \propto t^{2/3}, \qquad (4.5)$$

which is valid when $E \ll Zr^{-1}$. This can then be consistently inserted in (4.1b) (which itself is valid only when $\Delta r \ll r$). Letting $C_2{}^{\max}(E)$ be the maximum value of C_2 which leads to "double escape" at energy E, one finds that the corresponding solutions (4.1b) can be written

$$\Delta r_{\max}(E) \propto C_2{}^{(\max)}(E) t^{\frac{1}{2} + \frac{1}{3}\mu}. \qquad (4.1\text{c})$$

Applying (4.4b) then leads to the conclusion

$$C_2{}^{\max}(E) \propto E^{-\frac{1}{4} + \frac{1}{2}\mu}. \qquad (4.6)$$

In Eq. (4.6) the (quasi-ergodic) assumption has been made that all initial conditions for particles entering the emergent zone are essentially equally probable. From the remark above Eq. (4.4a) this then translates itself into

$$Q \propto E^{-\frac{1}{4} + \frac{1}{2}\mu}, \qquad (4.7)$$

which is Wannier's threshold law.[1]

The key assumption in this theory, in our opinion, is expressed in Eq. (4.6). We wish to show first that this assumption cannot be justified in a strictly classical theory of the whole ionization process. In that case the cross section emerges as a statistical average of events in which the orbital particle is initially bound. (Radiation damping is necessarily excluded.) The question one asks in ionization is what happens as the energy of the impinging particle increases, the characteristics of the bound particles remaining the same. *In other words, the variation with energy of the initial condition* (i. e., one particle incoming, the other particle bound) *does not satisfy the similarity principle*, Eqs. (4.4). But Newton's equations, in that case, cover the whole collision process. In other words, if the orbits corresponding to the solutions (4.1) be traced backward in time, it will be found that the overwhelming majority of them originate in trajectories in which the two electrons were originally approaching the nucleus from infinity, or in which if one of the particles is bound it will be bound with the wrong energy. These are initial conditions that must be excluded even from the most general type of distribution used to describe the real initial conditions. Thus we conclude that from a completely classical point of view the distribution of $C_2^{\max}(E)$ does not necessarily obey (4.6). It may be a very sensitive function of E (near threshold) and/or the result may not depend on $C_2(E)$ alone but on C_1 as well; it may also depend on the statistical distribution that one chooses to describe the initially bound orbits. It is, then, consistent with these arguments that classical Monte Carlo calculations do not reveal[18] the Wannier threshold law.

The same objection cannot *a priori* be raised against a quantum mechanical collision. For, in that case, the concept of an individual orbit does not apply throughout the collision process. Nevertheless the above consideration does raise the possibility that the way which particles emerge into the classical zone may also be a highly sensitive function of E. We believe that this in fact is the case, since even if one cannot speak in terms of orbits, the Hamiltonian does remain the same throughout the collision. The assumption would be more justified in our opinion in the problem of the threshold production, say, of two negatively charged hadrons by nucleon collisions with nuclei. In that case the short-range interactions only come into operation in the quantum mechanical zone, and they are so strong and complicated that they can legitimately be expected to make the final state completely oblivious to the initial state. Note that our approach to this problem completely avoids this assumption, but by the same token it cannot say anything about it.

In addition to this quasi-ergodic assumption there remains the question of the validity of the classical theory. This is a very difficult question which has not been definitively answered. We believe that in the ionization of atoms by electrons the theory does have some validity in the region $(\Delta r/r) \ll 1$. However, when the difference in the two radial distances gets large, then we believe that quantum effects (shielding) will have a profound role.[2] The present results tend to bear out this reservation.[18a]

Finally we mention the experimental situation. Although an experiment can never prove a threshold law, the experiment of McGowan and Clarke[19] has convincingly shown that there is some nonlinearity in the e – H ionization curve between threshold and 0.4 eV. For if there were not, then the measured position of the first resonance in e – H elastic scattering[20] would not coincide essentially with precision calculations,[21] which in our opinion cannot seriously be questioned. In the region 0.05 $< E < 0.4$ eV McGowan and Clarke find very good agreement with Wannier's $E^{1.127}$ law, but it is perhaps significant because the experiment is hardest there) that below 0.05 eV the yield curve does appear more nonlinear. Brion and Thomas[22] in e – He ionization also find a yield curve which appears to be more nonlinear than Wannier's law. Since the region of nonlinearity is much greater there, this may provide a better experimental test of the theory.

APPENDIX

In this Appendix we shall derive the normalization factor for a particle scattered in an attractive r^{-2} potential. We shall also estimate its effect on the ionization threshold.

The inelastically scattered wave satisfies the equation

$$\left[\frac{d^2}{dr^2} + \frac{|b_{Nj}|}{r^2} + k_N^2\right] f_{Nj}(r) = 0. \qquad \text{(A1)}$$

It is important that this equation exclude regions near the origin; this is evident from the general solution of (A1)[23]

$$f_{Nj}(r) = A r^{1/2} J_{i\alpha_{Nj}}(k_N r) + B r^{1/2} N_{i\alpha_{Nj}}(r), \qquad \text{(A2)}$$

which oscillates infinitely rapidly (and thus is unacceptable) as $r \to 0$. α_{Nj} is given by

$$\alpha_{Nj} = (|b_{Nj}| - \tfrac{1}{4})^{1/2} \equiv \alpha. \qquad \text{(A3)}$$

Using the asymptotic form of the Bessel function for $k_N r \gg \alpha_{Nj}$ in (A2) gives

$$\lim_{r\to\infty} f_{Nj}(r) = A\left(\frac{2}{\pi k_N}\right)^{1/2} \cos\left(k_N r - \frac{i\alpha\pi}{2} - \frac{\pi}{4}\right) + B\left(\frac{2}{\pi k_N}\right)^{1/2} \sin\left(k_N r - \frac{i\alpha\pi}{2} - \frac{\pi}{4}\right). \qquad \text{(A4)}$$

We demand that $r^{-1} f_{Nj}(r)$ be normalized to a plane wave, so that

$$\lim_{r\to\infty} f_{Nj}(r) = \frac{C}{k_N} \sin(k_N r + \delta), \qquad \text{(A5)}$$

where C is independent for k_N. Comparison of (A5) and (A4) shows that A and B are proportional to $k_N^{-1/2}$.

On the other hand, A and B must also be related to the solution for smaller values of r. To get this relation we must first rewrite (A2) in a region where $k_N r \ll \alpha_{Nj}$, but where the r^{-2} potential is still operative. The function $f_{Nj}(r)$ can there be approximated by the small argument expansion[24] of the Bessel functions. I. e., for $k_N r \ll \alpha_{Nj}$ but $r \geqslant r_0$

$$f_{Nj}(r) \cong A r^{1/2} (\tfrac{1}{2} k_N r)^{i\alpha} / \Gamma(1 + i\alpha) + B r^{1/2} / \sin(i\alpha\pi) \times \left[\left(\frac{k_N r}{2}\right)^{i\alpha} \frac{\cos(i\alpha\pi)}{\Gamma(1+i\alpha)} - \frac{(k_N r)^{-i\alpha}}{\Gamma(1-i\alpha)}\right]. \qquad \text{(A6)}$$

The radius at which the r^{-2} potential is no longer operative is defined as r_0. Within this radius we assume that we can represent the solution for whatever (in reality very complicated and nonlocal) potential does exist as

$$f_{Nj}(r)=\eta f(r). \tag{A7}$$

The quantity η is the desired normalization factor. It can be determined by equating the logarithmic derivative of (A6) and (A7) at $r=r_0$. One finds to an excellent approximation

$$\eta=r_0^{1/2}/f(r_0)[k_N(\tfrac{5}{4}-R_0r_0+R_0^2r_0^2)]^{1/2}\ , \tag{A8}$$

where $R_0\equiv[f'(r)/f(r)]_{r=r_0}$. (A9)

In order to estimate the effect of this on the ionization, it is necessary to have some idea of the size of r_0. A lower bound estimate of it is that radius at which the outer electron is comparable with the mean radius of the inner electron $\bar{r}_2$. (It cannot be smaller for then it would no longer be the outer electron.) But for a hydrogenic atom in the Nth state $\bar{r}_2\propto N^2$; thus it is clear that as N gets large, r_0 must also. Hence

$$\lim_{N\to\infty}\eta=|f'(r_0)|^{-1}(k_Nr_0)^{-1/2}\ . \tag{A10}$$

Before proceeding let us note that for a finite N the factor $k_N^{-1/2}$ in (A8) or (A10) is the same as one would have for a pure Coulomb wave. It is this factor which is directly responsible for the finite threshold behavior in electron-impact excitation of hydrogen. This simple fact which is the implicit basis of the original derivation of this result by Gailitis and Damburg[23] is somewhat obscure in their paper as a result of their very elegant and very general mathematical procedure.

To calculate the effect on the ionization we must replace $F_l(k_Nr_1)$ in (3.1) by $\eta f(r_1)$ in view of the fact that the dominant contribution to the matrix element comes from r_2 small and r_1 comparable with r_2. In this case the sum (3.4) must be extended from $j=1$ to $j=J_D$. Everything proceeds in complete analogy with the development after Eq. (3.1), and we again replace the sum over j in this case by J_D. The counterpart of Eq. (3.11) then becomes

$$Q_D\propto\int k_N[k_N^{1/2}N^2|f'(r_0)|r_0^{1/2}]^{-2}J_DN^3dw. \tag{A11}$$

Using Eq. (2.14) for J_D, we obtain

$$Q_D\propto\int dw/|f'(r_0)|^2r_0\ . \tag{A12}$$

In order to evaluate (A12) we must know how $f'(r_0)$ depends on r_0 and how r_0 depends on N. The only way that this can be done is to adopt a model which will hopefully be both manageable and realistic. We shall assume that for $r<r_0$, $f_{Nj}(r)$ sees a square well of depth $-V_0$. For r_0 we use half the estimate derived in Ref. 11 [Eq. (2.24)]

$$r_0\cong b_{Nj}/2\epsilon_{Nj}^{1/2}. \tag{A13}$$

For higher resonances of a given N and j, $2r_0$ gives a good estimate of the region in which the dipole potential operates and therefore characterizes the size of the state. For the lowest resonance the dipole potential alone does not exhaust the configuration space of the major part of the wave function. Equation (A13) amounts to saying that the more complicated potential extends over half of the dipole region. Calculations of Chen[25] are in remarkable agreement with this estimate.

ϵ_{Nj} is the binding energy of the state relative to Nth threshold energy. For ϵ_{Nj} we use the formula

$$\epsilon_{Nj}\propto N^{-(2+\xi)} \tag{A14}$$

with the limits,

$$0\leqslant\xi\leqslant1, \tag{A15}$$

indicating that ϵ_{Nj} remains between the Nth and $(N-1)$st level at the least $(\xi=1)$ to being Rydberg in nature at the most $(\xi=0)$. If we substitute (A14) into (A13), then using (2.15) we find

$$r_0\propto N^{3+\xi/2}. \tag{A16a}$$

Actual calculations for $v_{Nj}(r)$ for $N=5$, $j=2$ (cf. Fig. 2) show that $r_0\propto N^3$, and it is otherwise quite certain that $\xi=0$ cannot be exceeded as an estimate of r_0. For the purpose of the estimate, therefore, we shall take

$$r_0\propto N^3. \tag{A16b}$$

According to the model, the interior solution is

$$f_{Nj}(r)=\eta\sin Kr, \tag{A17a}$$

where $K=(v_0-\epsilon_{Nj})^{1/2}$. (A18)

From (A7) this means

$$f(r)=\sin Kr. \tag{A17b}$$

Thus the secular dependence of $f'(r_0)$ is clearly[14]

$$[f'(r_0)]_{\text{secular}}\propto K. \tag{A19}$$

To relate K to N we demand that $f(r)$ have N^2 nodes as is demanded by the orthogonality requirement (2.12). Actually (2.12) confines the nodes to a radius $\bar{r}_2\propto N^2$ where $v_{Nj}(r)$ overlap the radial functions $R_{Nl}(r_2)$ describing the inner electron. However, Fig. 2 shows that the amplitude of the inner oscillations are minuscule, and only when $r_1\cong r_0$ of Eq. (A16b) does the amplitude become sizable. The condition

$$Kr_0=N^2\pi \tag{A20}$$

replaces this by an evenly oscillating function of uniform amplitude throughout the whole region.

It follows then that

$$K\propto N^{-1}. \tag{A21}$$

One substitutes all of this into (A12) to get

$$Q_D \propto \int dw/N \propto \int_0^E w^{\frac{1}{2}}\; dw$$

or finally

$$Q_D \propto E^{3/2}\,. \tag{A22}$$

Strictly speaking this, as well as the foregoing extrapolations, should be augmented by inclusion of the $P\Psi$ part of the wave function, in the language of the Feshbach theory.[6] However, it is clear when working below threshold that this contribution has a scattered part which is a phase-shifted plane wave by construction. Thus it is known to contribute in the order $E^{3/2}$.

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