layer is very similar to the E in scale height, in maximum density of ionization, in the extent and symmetry of its diurnal variation, and perhaps in its behavior over longer periods. In case these ideas are correct, we must look for an explanation of the seasonal appearance and disappearance of the F_1 critical frequency in the distribution of ionization with height in the F_2 layer.

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The Calculation of the Coordinate Matrix Elements for Helium

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Formulae for the calculation of transition probabilities in an atom with two electrons are derived for transitions from discrete s to both continuous and discrete p-states.

I. INTRODUCTION

It is of interest, especially on account of its application to astrophysics, to investigate the influence which the mutual interaction of the two electrons in helium has on the matrix elements of the coordinates. The various perturbations, the coulomb interaction, the exchange, and the "polarization" all contribute to the energy. As a consequence, the chief quantum number, n, is no longer integral. These perturbations are taken together as the "Rydberg correction," δ, so that $n=[n]+\delta$. We assume here that the results of the energy calculation are known[1] and wish to calculate the coordinate matrix elements for variable n.[2] In order to find the matrix element for an atom, δ is taken from one of the calculated energies and the value of n is then substituted in our formulae.

The Rydberg correction is particularly large for s-states. We should therefore expect the greatest deviations from the hydrogen matrix elements for the transitions sp and these are accordingly treated here.

1. Transitions from discrete s to continuous p-states

The orbital eigenfunction Ψ, after splitting off from the spin function, must be either symmetric (para) or antisymmetric (ortho) in the electrons

$$\Psi=2^{-\frac{1}{2}}[\Psi_i(r_1)\Psi_a(r_2)\pm\Psi_i(r_2)\Psi_a(r_1)].$$

The inner electron is in the ground state

$$\psi_i=e^{-Zr/a},\quad a=\hbar^2/m_0e^2.$$

Z is the nuclear charge in the field of which the inner electron moves. For the outer electron moving in the reduced field z, we will assume that the eigenfunction Ψ_a may be expressed as the product of a radial function and a spherical harmonic function, $\Psi_a=\psi(r)\cdot Y_{lm}(\Theta,\Phi)$. If this is substituted in the expressions for the matrix elements of the coordinates, exactly the same selection rules and the same coefficients, depending only on l and m, as in the hydrogen matrix elements result.[3] Only the integrals depending on the radius are altered. If we denote with capital letters N, L, M the quantum numbers corresponding to the state with the higher azimuthal quantum number, $L=l+1$, and substitute for r the dimensionless quantity $\rho=2zr/a$, we obtain the expression $R_{nl}^{NL}\cdot a/2z$, which Gordon denoted by C.

For the (sp)-transitions

$$R_{nl}^{NL}=(II_{nN}\pm I_NI_n)\cdot[I_{NN}I(I_{nn}I\pm I_n^2)]^{-\frac{1}{2}}\quad(1,1)$$

where

$$I_{nN}=\int_0^\infty\psi_{n0}\psi_{N1}\rho^3d\rho;\quad I_{NN}=\int_0^\infty\psi_{N1}{}^2\rho^2d\rho;$$

[1] E. A. Hylleraas, Zeits. f. Physik 66, 453 (1930), 65, 209 (1930). H. A. Bethe, *Handbuch der Physik* [1], Vol. 24, p. 347.

[2] I have to thank E. A. Hylleraas for this suggestion. See also reference 5.

[3] W. Gordon, Ann. d. Physik 2, 1031 (1929).

$$I_{nn}=\int_0^\infty \psi_{n0}{}^2\rho^2 d\rho;\quad I=\int_0^\infty e^{-Z\rho/z}\rho^2 d\rho=2(z/Z)^3;$$

$$I_N=\int_0^\infty e^{-Z\rho/2z}\psi_{N1}\rho^3 d\rho;\quad I_n=\int_0^\infty e^{-Z\rho/2z}\psi_{n0}\rho^2 d\rho.$$

2. The approximate functions and their normalization

The difficulty lies in discovering suitable approximate functions for the discrete spectrum. In his earlier[4] calculation of the helium matrix elements, E. A. Hylleraas used the functions which the variation method yielded from the energy calculation. Lately,[5] Hylleraas has used complex integrals in order to extend the eigenfunctions for integral n, the Laguerre polynomials, to arbitrary n. This method shows itself to be especially suitable for the calculation of the transitions to the continuum.

The differential equation for ψ, if we neglect the polarization[6] and assume that the inner electron effectively reduces the nuclear charge to ze, is

$$\rho^2\psi''+2\rho\psi'-(l(l+1)-\rho+\rho^2/4n^2)\psi=0,\quad (2,1)$$

which is satisfied by

$$\psi(\rho)=\rho^l n^{-2l-1}(2\pi i)^{-1}\int e^{-\rho(1-2\zeta)/2n}\times(1-\zeta)^{l+n}\zeta^{l-n}d\zeta,\quad (2,2)$$

if the path of integration is taken so that at both ends

$$(1-\zeta)^{l+1+n}\zeta^{l+1-n}e^{-\rho(1-2\zeta)/2n}\quad (2,3)$$

has the same value.

For the discrete s-states, following Hylleraas, we take the path from $\zeta=-\infty$ round $\zeta=0$ back to $\zeta=-\infty$, whereby (2, 3) vanishes so long as $\rho>0$. If we let $\zeta=s/(1+s)$ and integrate by parts

$$\psi_n(\rho)=n(2\pi i\rho)^{-1}\int_{-\infty}^{(0,+)} e^{-\rho(1-2\zeta)/2n}\times(1-\zeta)^{n-1}\zeta^{-n-1}d\zeta$$
$$=n(2\pi i\rho)^{-1}\int_{-1}^{(0,+)} e^{-\rho(1-s)/(1+s)2n}s^{-n-1}ds.\quad (2,4)$$

ψ_n does not fulfill the boundary conditions at $\rho=0$, but can be used as an approximate function for the outer electron for the calculation of the matrix elements, as the deviation from the exact solution in the region $\rho=0$ contributes very little to the matrix integral I_{nN}.

The normalizing integral is easily found. It is

$$I_{nn}=2n^3\{1-[\Psi'(n)-(1/n)+(1/2n^2)]\times(\sin n\pi)^2/\pi^2\}.\quad (2,5)$$

The expansion of $\Psi'(n)=d^2/dn^2\log\Gamma(n)$ in reciprocal powers of n is[7] $\Psi'(n)=(1/n)-(1/2n^2)+(1/6n^3)-(1/30n^5)+\cdots$ so that the coefficient of $(\sin n\pi)^2$ is small compared with unity.

The interaction integrals for large, real quantum numbers are proportional to n^{-3} and vanish at the boundary of the continuum. The eigenfunctions of the continuum are hydrogen eigenfunctions but in the reduced field, z. We can take them from Sommerfeld,[8] remembering that his ρ is our ρ/n

$$\psi=\frac{\Pi(n+l)}{\Pi(n-l-1)}i^l n^{-l-1}R$$
$$=\frac{\Pi(n+l)}{\Pi(n-l-1)}\rho^{-l-1}(2\pi i)^{-1}\oint(x+\tfrac{1}{2})^{n-l-1}\times(x-\tfrac{1}{2})^{-n-l-1}e^{-\rho x/n}dx.\quad (2,6)$$

Sommerfeld gives for the normalizing integral

$$\int_0^\infty R^2r^2dr=\frac{\pi}{2}k_s{}^{-2}e^{-\pi|n|}|\Gamma(n+l+1)|^{-2}(an^2/z);\quad k_s=z/|n|a.$$

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[4] E. A. Hylleraas, Zeits. f. Physik **106**, 395 (1937).
[5] E. A. Hylleraas, Archiv f. Math. og Natv. **48**, No. 4 (1945).
[6] We take account of the polarization approximately as it is included in $n=[n]+\delta$.
[7] Jahnke-Emde, *Funktionentafeln* (B. G. Teubner, Leipzig, 1938), p. 20.
[8] A. Sommerfeld, *Atombau und Spektrallinien II* (Friedrich Vieweg und Sohn, Braunschweig, 1938), p. 121, Eq. (28). The eigenfunction ψ is also given directly from our Eq. (2.2) by integrating by parts $(2l+1)$ times over the closed path about $\zeta=0$ and $\zeta=1$.

The last factor appears when we normalize for the quantum number interval $dn=1$.

The principal quantum number of the continuum is purely imaginary and we put $N=i\nu$, $\nu=(2m_0E)^{-\frac{1}{2}}\hbar z/a$, where E denotes the energy of the free electron.

Hence, for the p-state

$$I_{NN}=2\nu(\nu^2+1)(1-e^{-2\pi\nu}) \qquad (2,7)$$

and with $x=\eta+\frac{1}{2}$

$$\psi_N=(N^2-1)N\rho^{-2}(2\pi i)^{-1}\oint_{(-1,0)}(1+\eta)^{N-2} \times\eta^{-N-2}e^{-\rho(1+2\eta)/2N}d\eta. \qquad (2,8)$$

3. The matrix integral I_{nN}

The integral I_{nN} is first integrated over ρ

$$I_{nN}=nN^2(N^2-1)(2\pi i)^{-2}\int_{-\infty}^{(0+)}(1-\zeta)^{n-1}\zeta^{-n-1} \times\oint_{(-1,0)}(1+\eta)^{N-2}\eta^{-N-2}(\eta-\eta_0)^{-1}d\eta d\zeta. \qquad (3,1)$$

The integral with respect to η is equal to the negative residue at the pole

$$\eta_0=-\tfrac{1}{2}+N(2\zeta-1)/2n.$$

The transformation $2\zeta=1-1/y$ together with the abbreviation

$$f=n\log\frac{1+y}{1-y}-N\log\frac{1+ky}{1-ky}$$

$$=n\log\frac{1+y}{1-y}-2\nu\arctan(ny/\nu);$$

$$k=n/N=n/i\nu \qquad (3,2)$$

gives

$$I_{nN}=2^5n^5(1-1/N^2)e^{in\pi}(2\pi i)^{-1} \times\int_0^{(1+)}e^fy^4(1-y^2)^{-1}(1-k^2y^2)^{-2}dy. \qquad (3,3)$$

Integrating by parts

$$I_{nN}=-8n^2(1-k^2)^{-2}\{2(1-k^2)(\sin n\pi)/\pi +G_2+2nG_1+G_0\} \qquad (3,4)$$

where

$$G_0=-(\sin n\pi)/\pi,$$

$$G_j=e^{in\pi}(2\pi i)^{-1}\int_0^{(1+)}y^{-j}\frac{de^f}{dy}dy;\quad j=0,1,2. \qquad (3,5)$$

This form of the integrand suggests the introduction of f as a new variable.[9]

In order to calculate G_j we deform the path of integration so that it passes through the regular point $y=\infty$; in fact, we put $y=re^{-i\pi/3}$ along the path from 0 to ∞ and $y=re^{+i\pi/3}$ along the path back to 0. Then

$$G_j=\frac{1}{\pi}\lim_{r\to\infty}Re\left\{ie^{-in\pi}\int_0^{y=r\exp(i\pi/3)}y^{-j}\frac{de^f}{dy}dy\right\}. \qquad (3,6)$$

We expand f in powers of y and split up the coefficient of the lowest power, $f=-\frac{2}{3}n(1-k^2)\varphi$. For the integrals G_j we require y^{-1} and y^{-2} as power series in φ.

We let

$$y^{-1}e^{i\pi/3}=\frac{1}{r}=\sum_{p=0}^{\infty}a_p(e^{2i\pi/3}(1+k^2)/5)^p\varphi^{(2p-1)/3}$$

and

$$y^{-2}e^{2i\pi/3}=\frac{1}{r^2}=\sum_{p=0}^{\infty}b_p(e^{2i\pi/3}(1+k^2)/5)^p\varphi^{(2p-2)/3} \qquad (3,7)$$

where a_p, b_p are coefficients to be determined later. Then

$$G_1=\frac{1}{\pi}\sum_{p}^{\infty}a_p\Pi\left(\frac{2p-1}{3}\right)[(1+k^2)/5]^p \times[2n(1-k^2)/3]^{(1-2p)/3}\sin(-n-\tfrac{1}{3}+2p/3)\pi,$$

$$G_2=\frac{1}{\pi}\sum_{p=0}^{\infty}b_p\Pi\left(\frac{2p-2}{3}\right)[(1+k^2)/5]^p \times[2n(1-k^2)/3]^{(2-2p)/3}\sin(-n-\tfrac{2}{3}+2p/3)\pi. \qquad (3,8)$$

4. The calculation of the coefficients a_p, b_p

The most convenient relation for the calculation of a_p, b_p is

$$3\frac{d}{d\varphi}y^{-1}=(1-1/y^2)(k^2-1/y^2) \qquad (4,1)$$

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[9] Method of steepest descent.

TABLE I. Table of coefficients from the recursion formula (4, 4).

	$1\cdot$	$+a_1\cdot$	$+(a_2)^2\cdot$	$+(a_2)^3\cdot$	$+(a_2)^4\cdot$	$+(a_2)^5\cdot$
$a_2=$	0	1				
$a_3=$	0.11111111	−0.22222222				
$a_4=$	−0.11111111	−0.14141414	−0.54545455			
$a_5=$	0	−0.35431235	−0.24941725			
$a_6=$	−0.01975309	0.13029440	0.00676854	0.16969697		
$a_7=$	0.03209877	0.08669704	0.60214615	0.44129988		
$a_8=$	0	0.15052357	0.21678623	0.48512744	0.09073510	
$a_9=$	0.00463779	−0.06659891	−0.02767115	−0.35543989	−0.17129693	
$a_{10}=$	−0.01039911	−0.04400100	−0.44506038	−0.70035860	−0.80378893	−0.14795090
$a_{11}=$	0	−0.06435739	−0.14151900	−0.63408920	−0.54310902	−0.27641329
	$1\cdot$	$+a_2\cdot$	$+(a_2)^2\cdot$	$+(a_2)^3\cdot$	$+(a_2)^4\cdot$	$+(a_2)^5\cdot$
$b_2=$	1	2				
$b_3=$	0.22222222	1.55555556				
$b_4=$	0	−0.72727273	−0.09090909			
$b_5=$	−0.22222222	−0.76923077	−2.03418803			
$b_6=$	−0.02716049	−0.71964085	−0.71874299	−0.75151515		
$b_7=$	0	0.45194022	0.45084327	0.96558344		
$b_8=$	0.07654321	0.38762433	2.14170974	2.13151380	0.81838480	
$b_9=$	0.00488601	0.34851639	0.65085535	1.95543443	0.91814678	
$b_{10}=$	0	−0.23956751	−0.44040667	−1.85259927	−1.16922010	−0.29955557
$b_{11}=$	−0.02793128	−0.18833842	−1.60090500	−3.14552213	−4.50545115	−1.79771769

which, together with

$$b_p=\sum_{q=0}^{p} a_q a_{p-q} \qquad (4,2)$$

give

$$a_0=1;\quad a_1=1;\quad a_2=(1-4k^2)(4-k^2)(1+k^2)^{-2}/7;$$
$$b_0=1;\quad b_1=2;\quad b_2=1+2a_2 \qquad (4,3)$$

and the following coefficients from the recursion formulae

$$\begin{aligned}(2p+3)a_p&=5b_{p-1}-\sum_{q=1}^{p-1}(b_q b_{p-q}+2a_q a_{p-q});\\ b_p&=2a_p+\sum_{q=1}^{p-1}a_q a_{p-q}.\end{aligned} \qquad (4,4)$$

The next coefficients are given as polynomials in a_2 in Table I. The series (3, 8) for G_1 and G_2 are asymptotic series in which the terms decrease rapidly after the first. Only for very small ν, i.e., for high energies of the free electron, is a greater number of terms necessary.

5. The exchange integrals I_N and I_n

The integral I_N can easily be calculated, as the path of integration for η in (2, 8) is closed. We integrate for ρ, put $2\eta=y-1$ and $m=z/Z$ and integrate by parts.

$$I_N=-2^6N^3(N^2-1)(2\pi i)^{-1}\oint_{(-1,\,+1)}(y+1)^{N-3}(y-1)^{-N-3}(2y+N)(y-y_0)^{-1}dy. \qquad (5,1)$$

The path of integration can be contracted round the pole $y_0=-N/m=-i\nu/m$. Then

$$I_N=4^3N^4(N^2-1)(N-m)^{N-3}(N+m)^{-N-3}(m-2)m^5 \qquad (5,2)$$

or

$$I_N=4^3\nu^4(\nu^2+1)(\nu^2+m^2)^{-3}(m-2)m^5\exp[-2\nu\arctan(m/\nu)]. \qquad (5,3)$$

The integral I_n is integrated first over ρ and then by parts

$$I_n=4n^2m^2(n^2-m^2)^{-1}\Big\{[2n(1-m)(n+m)^{-1}-1](\sin n\pi)/\pi$$
$$+4mn^2(1-m)(n+m)^{-2}(2\pi i)^{-1}\int_{-1}^{(0+)}s^{-n}(1+st)^{-1}ds\Big\};\quad t=(n-m)/(n+m). \qquad (5,4)$$

Expanding the denominator and integrating round a unit circle

$$I_n=4n^2m^2(n+m)^{-3}\left\{n+m-2mn+\frac{4m^2n}{1-n}+4mn^2(1-m)(n+m)^{-1}\sum_{p=1}^{\infty}t^{p-1}/(p+1-n)\right\}(\sin n\pi)/\pi. \quad (5,5)$$

This series converges rapidly only when t is small compared with 1. As $m=z/Z<1$, generally $n\gg m$. In order to find an expansion in powers of n^{-1} we transform the pole to 0 by putting $st=y-1$ and deform the path of integration so that it runs from $y=1-t$ in the negative imaginary half-plane to $y=-\infty$ and back in the positive imaginary half to $1-t$. Then

$$\int_{-1}^{(0+)}s^{-n}(1+st)^{-1}ds=-t^{n-1}\left(\cos n\pi\oint(1-y)^{-n}dy/y+2i\sin n\pi\int_{-\infty}^{1-t}(1-y)^{-n}dy/y\right).$$

The first integral is given by contracting both paths about the pole and has the value $2\pi i$. Substituting $y=x/(n+m)$ in the second integral

$$\int_{-\infty}^{1-t}(1-y)^{-n}dy/y=\int_{-\infty}^{2m}e^x/x\exp[-x-n\log(1-x/(n+m))]dx.$$

Expanding the second exponential function in powers of $1/n$ and integrating term by term, we have finally

$$I_n=-4m^2n^2(n^2-m^2)^{-1}(\sin n\pi)/\pi-16m^3n^4(1-m)(n^2-m^2)^{-2}t^n$$
$$\times\{\cos n\pi+[\langle Ei\rangle_{\mathrm{Av}}(2m)+e^{2m}C](\sin n\pi)/\pi\},$$
$$C=-\tfrac{1}{2}m+(2m-1)/12n^2+(20m^4-4m^3+6m^2-6m+3)/90n^4+\cdots. \quad (5,6)$$

In the case of helium, $Z=2$, $m=z/Z=\frac{1}{2}$, so that

$$I_n=-4n^2(4n^2-1)^{-1}(\sin n\pi)/\pi-16n^4(4n^2-1)^{-2}t^n$$
$$\times\{\cos n\pi+[\langle Ei\rangle_{\mathrm{Av}}(1)-e+(e/40n^4)+\cdots](\sin n\pi)/\pi\}, \quad (5,7)$$

to an accuracy of over 0.01 percent for all $n>1.5$.

II. TRANSITIONS FROM DISCRETE s- TO DISCRETE p-STATES

We wish to investigate the junction between the continuous and the discrete spectrum. We shall then be able to neglect the Rydberg correction for the discrete p-state in comparison with its much greater value for the s-state, so that N is a whole number. With this assumption E. A. Hylleraas[5] has calculated the matrix integrals. His series are, however, differently constructed so that an immediate comparison is not easily made. We shall therefore indicate shortly how our formulae for the discrete spectrum are to be altered.

As approximate function for the discrete p-state we use (2, 2) in which, as N is integral, the path of integration can be taken round $\zeta=0$ and $\zeta=1$. Integrating by parts three times gives (2, 8). The normalizing integral is

$$I_{NN}=2N(N^2-1). \quad (6,1)$$

At the boundary of the continuum $N\rightarrow\infty$, $\nu\rightarrow\infty$, Eqs. (6, 1) and (2, 7) become identical.

Equations (5, 1) and (5, 2) for I_N are always valid because $N>1>m$. Our expression for the matrix integral I_{nN} can be taken over unchanged so long as $N\gg n$.

The matrix elements of the continuum therefore join continuously with those for the discrete spectrum.

When $N \ll n$ the path of integration is taken along $y = re^{\pm 2\pi i/3}$. This gives the same formulae (3, 8) for G_j; instead of $(1-k^2)^{(j-2p)/3} \cdot \sin[-n-(j-2p)/3]\pi$ we now have

$$(k^2-1)^{(j-2p)/3} \cdot \sin[-n-(2j+2p)/3]\pi.$$

The asymptotic series (3, 8) for G_1 and G_2 become useless as N approaches n. We shall therefore, for the sake of completeness, also give expressions which can be used when $N \approx n$.

We substitute $y=(1+s)/(1-s)$ in Eq. (3, 5) and expand the integral in powers of $\epsilon=(N-n)/(N+n)$. Then

$$G_2+G_0=2n\epsilon(A+B)(\sin n\pi)/\pi; \quad G_1=n\epsilon(A-B)(\sin n\pi)/\pi$$

and

$$I_{nN}=16n^2N(1+k)^{-3}\{(1+k)^2+n(A+B)+n^2(A-B)\}(\sin n\pi)/(n-N)\pi,$$

where

$$A=-(N+n)^{-1}S_0{}^1+\sum_{p=1}^{N} S_{p-1}{}^0\epsilon^{p-1}/(N-n-p)+\sum_{p=1}^{\infty} S_0{}^{p+1}(-\epsilon)^{p+1}/(N-n+p),$$

$$B=+(N+n)^{-1}S_1{}^0+\sum_{p=1}^{N-2} S_{p+1}{}^0\epsilon^{p+1}/(N-n-p)+\sum_{p=1}^{\infty} S_0{}^{p-1}(-\epsilon)^{p-1}/(N-n+p).$$

For

$$S_a{}^b=\sum_{q=0}^{N-1-a}\binom{N-1}{a+q}\binom{N+b+q}{N}(-\epsilon^2)^q,$$

we have the following recursion formulae

$$(N+b)\cdot[S_0{}^{b-1}+\epsilon^2 S_0{}^{b+1}]=S_0{}^b\cdot[(1+\epsilon^2)b+2N\epsilon^2],$$

$$(N-a)\cdot[S_{a-1}{}^0+\epsilon^2 S_{a+1}{}^0]=S_a{}^0\cdot[(1+\epsilon^2)a-2N\epsilon^2],$$

and

$$S_0{}^1-S_1{}^0=2S_0{}^0, \quad S_{N+p}{}^0=S_N{}^0=0; \quad S_{N-1}{}^0=1.$$

In order to calculate transitions from discrete p- to continuous s-states the approximate function for the p-state must be changed, as also for transitions with higher l. The matrix integral I_{nN} can be calculated as the corresponding integrals G_j can be reduced to our G_1 and G_2 by integration by parts. But the approximate function can then no longer be normalized.

Investigation and also numerical calculations along these lines are in progress.

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