

therefore is clearly that our modified line is due to the helium only. These considerations render unnecessary a control experiment with vacuum in place of helium.

Huge difference between the electron velocities in the solid and vapor states

Before closing we wish to call especial attention to the enormous difference between the electron velocities in the solid state and those in the vapor state which the results of this paper, together with our previous work, clearly indicate must exist. In carbon, for example, the maximum of the electron velocity distribution curve is displaced to velocities 60 percent higher than in the free atom, an excess which our present results force us to take seriously as a real effect. See Fig. 8, reproduced from one of our papers.¹⁷

This speeding up of the electrons applying, let us say, to four electrons per atom as in carbon represents an enormous positive increase in electronic kinetic energy in the solid state as compared to the vapor state. For carbon we compute the increase to be in excess of 3×10^9 joules per gram. There is of course an even slightly greater *fall* in electron potential energy

caused by the proximity of positive nuclei in the solid state so that the net energy of the solid state is lower than the vapor state by the familiar required amount. Thus this profound difference between the two states is entirely masked in all conceivable methods of observation save the broadening of the modified line which alone affords a direct measurement of the electron velocities in the scattering material independent of their potential energy.

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The Shape of the Compton Line for Helium and Molecular Hydrogen

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By using variation functions which take into consideration the instantaneous interaction of the electrons, momentum distribution functions and intensity distributions in the Compton line are computed for helium and molecular hydrogen, neglecting small relativity and binding corrections. The half-value breadths are expressed in terms of $l/2\lambda^*$ where l is the wave-length displacement from the center of the shifted line and $2\lambda^* = (\lambda_1^2 + \lambda_c^2 - 2\lambda_1\lambda_c \cos \chi)^{1/2}$. λ_1 and λ_c are the primary and scattered wave-lengths and χ the scattering angle. The absolute breadth of the line may therefore be computed for any λ_1 and χ . For helium and molecular hydrogen the values of $l/2\lambda^*$ at half-maximum are 10.8 and 8.5, respectively.

INTRODUCTION

THERE have been many theoretical investigations of the shape of the Compton line differing from one another both in the treatment of the scattering process itself and in

the electronic configuration assumed to exist before scattering has occurred.^{1, 2} However, in no

¹J. W. M. DuMond, *Rev. Mod. Phys.* **5**, 1 (1933); *Phys. Rev.* **33**, 643 (1929).

²G. E. M. Jauncey, *Phys. Rev.* **25**, 314, 723 (1925); P. A. Ross and Paul Kirkpatrick, *Phys. Rev.* **45**, 223

calculation has the interaction of the electrons found suitable representation, for the Hartree functions or hydrogen-like wave functions with screening constants which have heretofore been used introduce only an average perturbing effect of the electrons upon one another. Since computations of the Compton line shape have been most successful for gases, it is natural when attempting a more rigorous investigation to turn to the simplest elementary gases containing two electrons, namely helium and molecular hydrogen. For these substances it is not necessary to depend upon the Hartree or screening-constant-type wave function since variation functions containing interaction terms explicitly have been developed, the most accurate of which lead to energy values for the ground state which are correct within experimental error. Line shapes for helium and molecular hydrogen are here computed from some of the less accurate of these variation functions which nevertheless approximate the true wave functions much more closely than do the Hartree or the hydrogen-like screening-constant type. By reason of the greater accuracy possible in these calculations as compared to calculations on other gases or solids, the line shapes for these two gases probably offer the best opportunity to compare in a quantitative fashion theory and experiment.³

GENERAL METHOD

The variation function chosen to describe the He or H₂ system is here represented by $\phi(r_1, \vartheta_1, r_2, \vartheta_2)$, where r_1, ϑ_1 are polar coordinates of the first electron, r_2, ϑ_2 of the second electron with respect to the same origin. Azimuthal angles do not appear in any of the variation functions used. $A(P_1, \Theta_1; r_2, \vartheta_2)$, the mixed wave function in the polar coordinates of the first electron in momentum space and the position coordinates of the second electron, can be obtained from this ϕ by the following Dirac transformation,

(1934); F. Bloch, Phys. Rev. **46**, 674 (1934); F. Schnaidt, Ann. d. Physik **21**, 89 (1934); W. Franz, Zeits. f. Physik **90**, 623 (1934); **95**, 652 (1935); G. Burkhardt, Ann. d. Physik **26**, 567 (1936); Kirkpatrick, Ross, and Ritland, Phys. Rev. **50**, 928 (1936).

³ The complete experimental results of DuMond and Kirkpatrick (Phys. Rev., this issue) on scattering in He demonstrate the feasibility of such a comparison and its importance in determining the position of the shifted line accurately.

$$A(P_1, \Theta_1, r_2, \vartheta_2) = h^{-3} \int_{r_1=0}^{\infty} \int_{\vartheta_1=0}^{\pi} \int_{\varphi_1=0}^{2\pi} \exp[-(2\pi i/h)\mathbf{P}_1 \cdot \mathbf{r}_1] \cdot \phi(r_1, \vartheta_1, r_2, \vartheta_2) r_1^2 \sin \vartheta_1 dr_1 d\vartheta_1 d\varphi_1 \quad (1)$$

(No azimuthal angle enters in A as none enters in ϕ .) Here, \mathbf{P}_1 and \mathbf{r}_1 are the vectors whose end-points lie at (P_1, Θ_1) , (r_1, ϑ_1) , respectively. All the transformation integrals which must be evaluated may be written down immediately by using the general expression for the momentum wave functions of a hydrogenlike atom, T_{nlm} , given by Podolsky and Pauling.⁴ Those functions which will be used here are:

$$\begin{aligned} T_{100} &= (1 + \zeta_1^2)^{-2}, \\ T_{200} &= 2(1 + \zeta_1^2)^{-2}(\zeta_1^2 - 1)/(\zeta_1^2 + 1), \\ T_{300} &= (1 + \zeta_1^2)^{-2} \left[4 \left(\frac{\zeta_1^2 - 1}{\zeta_1^2 + 1} \right) - 1 \right], \\ T_{210} &= -4i \cos \theta \frac{\zeta_1}{(1 + \zeta_1^2)^3}, \end{aligned} \quad (2)$$

where $\zeta_1 = 2\pi P_1 a_0 / Z' h$, Z' = effective nuclear charge and a_0 = radius of first Bohr orbit in hydrogen, the subscripts in T_{nlm} referring to the quantum numbers, n, l, m . ζ_1 will be used in place of P_1 , in the explicit functions of P_1 developed later for He and H₂. The momentum distribution function $B(P_1, \Theta_1)$ can now be found by integrating the modulus squared of $A(P_1, \Theta_1; r_2, \vartheta_2)$. Thus

$$B(P, \Theta) = 2\pi \int_{r_2=0}^{\infty} \int_{\vartheta_2=0}^{\pi} AA^* r_2^2 \sin \vartheta_2 dr_2 d\vartheta_2. \quad (3)$$

The subscripts have been dropped in $B(P, \Theta)$ for the electrons contribute equally to the momentum.

Since for this case of scattering by field-free gases, all orientations of the molecule are equally probable, the function $B(P, \Theta)$ must be averaged over the angle Θ to obtain the radial momentum distribution function, $C(P)$:

$$C(P) = \int_{\Theta=0}^{\pi} B(P, \Theta) \sin \Theta d\Theta. \quad (4)$$

⁴ Boris Podolsky and Linus Pauling, Phys. Rev. **34**, 109 (1929).

TABLE I. Variation functions for the normal He atom.

	Z'	c_2	c_5	$E - (\text{UNITS } R_{\text{He}}hc)$	% ERROR
1	1.6875	0	0	5.695	1.93
2	1.850	0	0.112	5.755	0.91
3	1.69	0.142	0	5.754	0.92
4	1.822	0.126	0.089	5.784	0.40

DuMond¹ has shown that the shape of the Compton line can be computed from such a momentum distribution function or *vice versa*, the formula for the intensity y as a function of wave-length displacement l from the center of the shifted line being

$$y = k \int_{l=l}^{\infty} l^{-1} C \left(\frac{l}{2\lambda^*} \right) dl, \quad (5)$$

in which $l = \lambda_2 - \lambda_1 - (h/mc)(1 - \cos \chi)$, $2\lambda^* = (\lambda_c^2 + \lambda_1^2 - 2\lambda_1\lambda_c \cos \chi_1)^{1/2}$, $\lambda_c = \lambda_2$ for $l=0$. λ_1 and λ_2 are initial and scattered wave-lengths and χ is the scattering angle. $C(P)$ has been replaced by $C(l/2\lambda^*)$ where

$$\frac{l}{2\lambda^*} = \beta = \frac{v}{c} = \frac{P}{mc} \quad \zeta = \frac{l}{2\lambda^*} \cdot \frac{1}{\alpha Z'}$$

α being the fine structure constant. Since the constant of integration k is arbitrary, all constant factors multiplying ϕ , A , B , and C are omitted.

It should be mentioned that DuMond's formula for the intensity distribution in the modified line does not consider the generally small effect due to binding and relativistic corrections. However, for the case of scattering from helium and the hydrogen molecule, binding and relativistic corrections to the shape are less than the error in the calculations due to the use of a variation function as an approximation to the true wave function. The error produced in the half-width itself is negligible since the corrections to the intensity corresponding to a given absolute value of l are nearly equal, though of opposite sign, on either side of the maximum.

Scattering from helium

The variation functions developed by Hylleraas⁵ for He are of the form

$$\phi = \sum_{nlm} c_{nlm} e^{-Z's} s^n t^l u^m \quad (6)$$

(l even)

in which $s = (r_1 + r_2)/a_0$, $t = (r_1 - r_2)/a_0$, $a_0 u = r_{12}$ = interelectronic distance, a_0 = radius of first Bohr orbit. Since a ϕ which involves the first power of u cannot be transformed in finite terms to the mixed wave function, variation functions which may be represented by

$$\phi = e^{-Z's} (1 + c_2 t^2 + c_5 u^2)$$

are used here. In Table I appear the four variation functions of this type together with the energy values to which they lead and the percentage difference from the true value. $E = -78.605 \text{ eV} = -5.8074 R_{\text{He}}hc$. The first of these is due to Kellner⁶ and is a hydrogen-like screening constant type function. The second is due to Hylleraas⁷ and the third and fourth have been developed by the author using Hylleraas' formulae.⁵ The terms in u^2 were included in an effort to compensate for the missing linear u term which is primarily responsible for the accuracy of Hylleraas' energy calculations. The third function describes the actual electronic system well since it represents a He atom with electrons in two different orbits with effective nuclear charges 2.15 and 1.19 corresponding to almost complete shielding of the outer one and slight negative shielding of the inner one. The second function, in comparison, although it now introduces the interelectronic interaction, represents this interaction as being much stronger than is actually the case. Consequently, of the two functions, the third probably corresponds more closely to the actual state of the system although the energy E calculated from the two functions is about the same. To check the effect of adding further integrable terms, values of E resulting from many different combinations of u^2 , u^4 , t^2 , t^4 , s , s^2 were computed. The most accurate value of the energy obtained in this way was only 0.1 percent better than the fourth variation function above. In view of the rapidly increasing complexity of the algebra entering into the evaluation of the integrals, it was not considered that the inclusion of further terms

⁵ Egil A. Hylleraas, *Skrifter det Norske Vid.-ak. Oslo, I Nat. Naturw. Klasse* 1932, p. 107.

⁶ G. W. Kellner, *Zeits. f. Physik* **44**, 91 (1927).

⁷ Egil A. Hylleraas, *Zeits. f. Physik* **54**, 347 (1929).

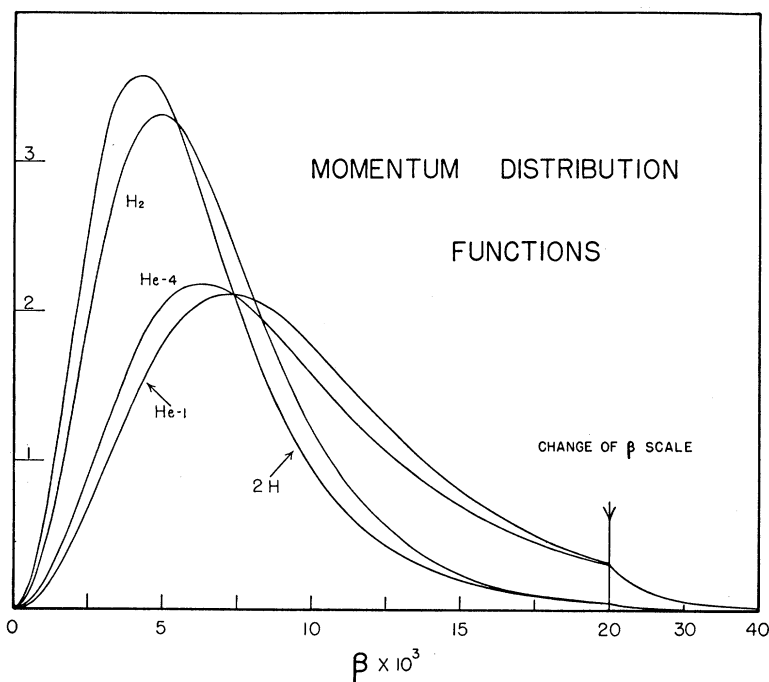


FIG. 1. Momentum distribution functions for helium and molecular hydrogen, normalized to the same area. The ordinates are in arbitrary units, the abscissae, in terms of $\beta = v/c$, the ratio of the velocity of an electron to that of light.

was justified. Furthermore, functions two and four lead to practically identical line shapes so that further terms would probably have little significance.

The necessary restriction of the exponents in the ϕ 's to even powers of u and l makes it possible to express these as linear functions of hydrogen-like $1s$, $2s$, $2p$, and $3s$ wave functions:

$$\phi = a_1 \psi_{100}(1Z') + a_2 \psi_{200}(2Z') + a_2' \psi_{210}(2Z') + a_3 \psi_{300}(3Z'). \quad (7)$$

Here a_1 , a_2 , a_2' , a_3 are quantities involving r_2 which are constants for the first integration and ψ_{nlm} is a hydrogen-like wave function for the first electron around a nucleus with charge $1Z'$, $2Z'$, \dots . From Eqs. (2) the mixed wave function then can be immediately written down as

$$A(\zeta_1, \Theta_1, r_2) = (1 + \zeta_1^2)^{-2} \left[a_1 + 2a_2 \frac{\zeta_1^2 - 1}{\zeta_1^2 + 1} + a_3 \left\{ 4 \left(\frac{\zeta_1^2 - 1}{\zeta_1^2 + 1} \right)^2 - 1 \right\} - 4i \cos \Theta_1 \frac{\zeta_1 \cdot a_2'}{1 + \zeta_1^2} \right] \quad (8)$$

and it becomes after integration over r_2 and Θ

$$C(\zeta) = (1 + \zeta^2)^{-4} \sum_{p=0}^4 D_p \left(\frac{\zeta^2 - 1}{\zeta^2 + 1} \right)^p, \quad (9)$$

$$y = (1 + \zeta^2)^{-3} \sum_{p=0}^4 E_p (1 + \zeta^2)^{-p}. \quad (10)$$

The coefficients D_p and E_p are polynomials in c_2/Z'^2 and c_5/Z'^2 . (For the first variation function $y \propto (1 + \zeta^2)^{-3}$ so that the polynomial in $(1 + \zeta^2)^{-1}$ may be considered to be a correction factor in the other expressions.) Consequently there should be expected a simple relationship between the *half-value breadths*, $\beta_{1/2}$, and the energy values corresponding to the different variation functions. A rough calculation of the line breadths of different many-electron systems may be made from a knowledge of the total energy E of the system alone if this energy has been computed by minimizing with respect to the effective nuclear charge Z' appearing in a hydrogen-like wave function with screening constants. This minimizing insures that the virial theorem hold so that the root mean square momentum and the

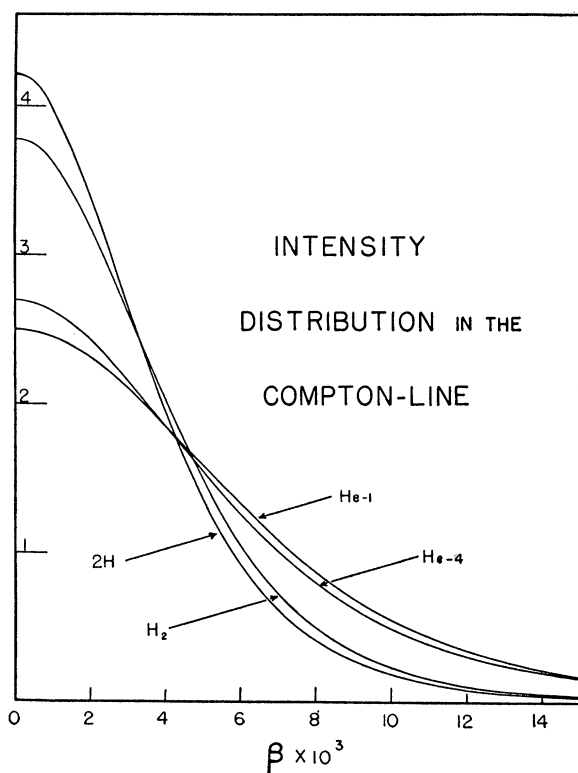


FIG. 2. Intensity distribution of the Compton line as a function of $\beta = l/2\lambda^*$ where l = displacement from the center of the shifted line, $2\lambda^* = (\lambda_1^2 + \lambda_c^2 - 2\lambda_1\lambda_c \cos \chi)^{1/2}$, λ_1 and λ_c being the initial and scattered wave-lengths and $\cos \chi$ the scattering angle. Ordinates are in arbitrary units and the curves are normalized to the same area.

half-value breadth may be taken as proportional to $(-E)^{1/2}$. For systems which may be considered to be hydrogen-like with all electrons in the same shell, this method will be exact since in this case $E \propto Z'^2$ and $\beta_{1/2}$ should be proportional to Z' , which is obviously true from a consideration of the simple form which y assumes for the hydrogen-like case.

A more accurate comparison may be made on the basis of the momentum distribution function, Fig. 1, for in general, $\beta_{1/2}$ corresponds closely in value to the most probable β . Thus, assuming

TABLE II. Half-value breadths.

$\beta_{1/2} \times 10^3$	Z'	$10^3 \times \beta_{1/2}/Z'$	$\beta_{1/2}$ calculated from most probable β
12.67	1.69	7.50	12.67
12.08	1.85	6.53	11.91
11.24	1.69	6.65	10.87
11.38	1.82	6.25	11.02

that $\beta_{1/2}$ as calculated from the first variation function is correct and that the half widths are directly proportional to the most probable β 's, approximate half widths are found which, with no attempt to adjust the constant of proportionality, fit to a few percent as is seen from the last column of Table II.

Since the variable is $\zeta = l/2\lambda^*Z'\alpha$ and the line shapes are plotted as functions of $l/2\lambda^* = \beta$, the half-value widths that should be compared are $\beta_{1/2}/Z'$. Values of $\beta_{1/2}$ (the half-value breadth) and $\beta_{1/2}/Z'$ are tabulated in Table II. If $(\beta_{1/2}/Z')$ is plotted as a function of the corresponding energy, it is seen to be an approximately linear function of the energy over a range which is long in comparison to the error in the energy computed from the fourth variation function and in consideration of the probable unreliability of the second variation function. Consequently, the extrapolated value of $(\beta_{1/2}/Z') = 5.99 \times 10^{-3}$ corresponding to $E = -5.8074 R_{He}hc$ may be assumed. By using the value $Z' = 1.818$ which occurs in the most accurate of the Hylleraas functions, the value $\beta_{1/2} = 10.8 \times 10^{-3}$ is then found, which is the best value that can be calculated from these variation functions. This method would not be valid if the constants did not enter into the variation function linearly.

In Fig. 2, y as a function of $l/2\lambda^* = \beta = v/c$ is plotted. From such a curve, the line shape for any scattering angle and any incident wave-length can be computed by a proper choice of λ^* (Eq. (5)). [For example, the half-width in He at $\lambda_1 = 710$ X.U., $\chi = 180^\circ$ is 15.8 X.U.] All curves are reduced to the same area since the total number of scattering electrons is constant. The two curves for He correspond to the first and fourth variation functions, and show clearly that

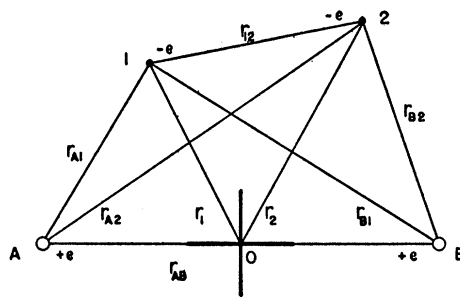


FIG. 3. Coordinates for the hydrogen molecule.

the line whose shape is computed from the more accurate function is narrower than the line derived from the simple hydrogen-like screening constant function.

Scattering from molecular hydrogen

A variation treatment for the hydrogen molecule has been carried out by James and Coolidge⁸ using terms in u to introduce the electronic interaction as Hylleraas did for He. However, the exponential of $(r_{A1} + r_{B1} + r_{A2} + r_{B2})/r_{AB}$, occurs in all the variation functions making impossible the evaluation of the transformation integral in finite terms. (See Fig. 3 for coordinates.) Consequently, a function of the ionic-polarization type studied by Weinbaum⁹ which permits the direct evaluation of all integrals but that for y has been chosen.

This variation function is

$$\phi = [u_{1s_A}(1) + \sigma u_{2p_A}(1)][u_{1s_B}(2) + \sigma u_{2p_B}(2)] + [u_{1s_A}(2) + \sigma u_{2p_A}(2)][u_{1s_B}(1) + \sigma u_{2p_B}(1)] \\ + c\{[u_{1s_A}(1) + \sigma u_{2p_A}(1)][u_{1s_A}(2) + \sigma u_{2p_A}(2)] + [u_{1s_B}(1) + \sigma u_{2p_B}(1)][u_{1s_B}(2) + \sigma u_{2p_B}(2)]\}, \quad (11)$$

in which $\sigma = 0.07$, $c = 0.176$, and $u_{1s_A}(1)$ represents a hydrogen-like $1s$ wave function for electron (1) about nucleus A which carries a charge Z' , etc. Thus

$$u_{1s_A}(1) = \exp(-Z'r_{A1}/a_0), \quad u_{2p_A}(1) = (r_{A1}Z'/a_0) \cos \vartheta_{A1} \exp(-Z'r_{A1}/a_0),$$

$$\vartheta_{A1} = \text{angle between } r_{AB} \text{ and } r_{A1}, \text{ measured from } r_{A1} \text{ to } r_{AB}.$$

The quantity r_{AB} , the internuclear distance, although not occurring in the variation function, enters in the calculation of the transformation integral. The experimental value, $0.7395A$, of r_{AB} is taken instead of 0.77 which corresponds to Weinbaum's function. This reduces the dissociation energy by a few percent, but gives a more accurate representation of the actual structure of the molecule. Z' is taken to be 1.19 since most variation functions of this general type lead to this value. ϕ may be rewritten as

$$\phi = a_A[u_{1s_A}(1) + u_{2p_A}(1)] + a_B[u_{1s_B}(1) + \sigma u_{2p_B}(1)]$$

in which

$$a_A = u_{1s_B}(2) + \sigma u_{2p_B}(2) + cu_{1s_A}(2) + c\sigma u_{2p_A}(2),$$

$$a_B = u_{1s_A}(2) + \sigma u_{2p_A}(2) + cu_{1s_B}(2) + c\sigma u_{2p_B}(2),$$

and a_A and a_B are therefore functions of the second electron's position alone. Since the transformation integral, Eq. (1), was expressed in terms of coordinates with but one origin, it is necessary to change its form slightly. Noting that ϕ splits up into two parts containing position variables with A and B as origin, and taking (x_{A1}, y_{A1}, z_{A1}) , (x_{B1}, y_{B1}, z_{B1}) to be rectangular Cartesian coordinates of the first electron with respect to A and B , the z -axis lying in the direction of the line AB , then the transformation integral becomes

$$A(P_{x_1}, P_{y_1}, P_{z_1}, x_{A2}, \dots, z_{B2}) = h^{-3/2} \left\{ a_A \exp[(\pi i/h)r_{AB}P_{z_1}] \int_{x_{A1}=0}^{\infty} \int_{y_{A1}=0}^{\infty} \int_{z_{A1}=0}^{\infty} \right. \\ \times \exp[-(2\pi i/h)\bar{P}_1 \cdot \bar{r}_{A1}] \cdot [u_{1s_A}(1) + u_{2p_A}(1)] dx_{A1} dy_{A1} dz_{A1} + a_B \exp[-(\pi i/h)r_{AB}P_{z_1}] \\ \left. \int_{x_{B1}=0}^{\infty} \int_{y_{B1}=0}^{\infty} \int_{z_{B1}=0}^{\infty} [u_{1s_B}(1) + u_{2p_B}(1)] \exp[-2\pi i/h)\bar{P}_1 \cdot \bar{r}_{B1}] dx_{B1} dy_{B1} dz_{B1} \right\}.$$

Since these integrals are exactly those for $1s$ and $2s$ hydrogen-like atoms, the mixed wave functions can at once be written out in polar coordinates by use of Eq. (2).

⁸ H. M. James and A. S. Coolidge, *J. Chem. Phys.* **1**, 825 (1933).

⁹ S. Weinbaum, *J. Chem. Phys.* **1**, 593 (1933).

$$A(P_1, \Theta_1, r_{A_2}, \dots, \vartheta_{B_2}) = [a_A \exp [(\pi i/h)r_{AB}P_1 \cos \Theta_1] + a_B \exp [-(\pi i/h)r_{AB}P_1 \cos \Theta_1]] [(1+\zeta_1^2)^2 - 4i\sigma\zeta_1 \cos \Theta_1] \cdot (1+\zeta_1^2)^{-3}. \quad (12)$$

Here ϑ_{A_1} = angle between r_{A_2} and r_{AB} , etc., while Θ = polar angle in momentum space of the first electron. Integrating over $r_{A_1} \dots \vartheta_{B_2}$ and Θ_1 , it follows that $A(P_1 \dots \vartheta_{B_2})$ becomes

$$c(\zeta) = (1+\zeta^2)^{-6} \left[(1+\zeta^2)^2 \left(1 + \frac{\lambda}{f\zeta} \sin(f\zeta) \right) + \frac{16}{3} \sigma^2 \zeta^2 + \frac{32\lambda\sigma^2}{f^2} \cos(f\zeta) + \frac{16\lambda^2\sigma^2}{f^3\zeta} (f^2\zeta^2 - 2) \sin(f\zeta) \right], \quad (13)$$

in which $\zeta = 2\pi P a_0 / Z' h$ as before, $f = Z' r_{AB} / a_0 = 1.67$, $\lambda = 2\mu(\mu c + 1 + c^2) / (4c/\mu + 1 + c^2) = 0.857$, where $\mu = 2(e' / f^2)(1 + \sigma^2)$ [polynomial in σ and f].

It is seen that in order to find y it is necessary to evaluate indefinite integrals of the form

$$\int_{\zeta}^{\infty} \frac{\sin(f\zeta)}{(1+\zeta^2)^n} d\zeta.$$

As a simplification, all integrals of this type were taken together and integrated graphically with an error of less than 1 percent. For purposes of comparison the resulting y curve was normalized to the same area as for two hydrogen atoms, or for a He atom and plotted with the He curves in Fig. 2.

Many other variation functions which it is possible to integrate have been studied by various investigators, but as each is of essentially different character from every other, and since the difference between any two is not merely a term in a polynomial as in the case of the helium, and the change in λ is consequently of a complicated nature, they would not provide basis for an extrapolation such as was carried out for helium. Accordingly it has not seemed worth while to calculate line shapes for these functions.

Interpolating on the y curve (Fig. 2), the

value $8.50 \times 10^{-3} = \beta_1$ is found for the half-value breadth of the line in H_2 . Since the half-width in atomic hydrogen is only 7.50×10^{-3} , the more accurate calculation leads to a broader line. This is not surprising in view of the change in the electronic configuration which occurs when two hydrogen atoms are brought together to form a molecule. The most important change which affects the momentum distribution is in the effective nuclear charge Z' . Because of the finite separation of the atoms and the interaction of the electrons with each other, Z' does not approach the value 2 as it would for independent electrons but increases to 1.19, according to the variation functions used. This Z' is near to the value 1.13 of the ratio of the two half-widths calculated above and would probably agree more closely if the assumption of the experimental value of r_{AB} had not invalidated the virial theorem in this case. It is interesting to note that the ratio of the most probable β 's calculated as in the case of helium is 1.12, checking closely the actual ratio of the half-widths.

The author is indebted to Dr. Linus Pauling for valuable criticisms during the course of this investigation.