

THE NORMAL STATE OF THE HYDROGEN MOLECULE

BY N. ROSEN

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

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ABSTRACT

The dissociation energy, moment of inertia, and fundamental vibration frequency are calculated for a normal hydrogen molecule by a variational method and are found to be 4.02 v, $4.66 \cdot 10^{-41}$ gm-cm², and 4260 cm⁻¹ as compared to the experimental values 4.42, $4.67 \cdot 10^{-41}$, and 4380, respectively. The calculation is carried through with the simplest possible improvements in the wave functions. In the appendix a number of integrals are listed and two tables of functions are included that may be useful to calculators.

I. INTRODUCTION

THE problem of calculating some of the properties of the normal hydrogen molecule by wave-mechanical methods has been hitherto successful qualitatively but not quantitatively. Thus Sugiura¹ by completing the calculations of Heitler and London² based on a first-order perturbation method, obtained 3.2 volts for the dissociation potential as compared to the experimental value, 4.4 volts. Wang,³ by using a variational method involving the introduction of a shielding constant, obtained 3.7 volts for this energy, which is a distinct improvement but still rather far from the goal. It is true that Condon⁴ obtained an almost exact agreement with experiment, but it is questionable as to whether one can call his method of doing this a straight-forward calculation. Eisenschitz and London,⁵ by carrying through a second order perturbation method, got 9.5 volts.

Similarly in the case of the two other quantities which are generally calculated at the same time as the energy, namely the equilibrium distance and the fundamental vibration frequency, the calculated results are not in very good agreement with the experimental values. If one surveys the available methods of calculating the quantities mentioned, it is at once evident that the only method for getting quantitative results is that based on the use of a variational principle, because the wave equation for this case cannot be solved exactly, and because solving it by the perturbation method is not to be trusted, as is shown by the fact that the second-order perturbation calculation gave a much worse result than the first-order calculation. In using the variational method one has the comforting assurance that one cannot go astray. If one starts with wave functions of sufficient complexity and having a large

¹ Sugiura, *Zeits. f. Physik* **45**, 484 (1927).

² Heitler and London, *Zeits. f. Physik* **44**, 455 (1927).

³ Wang, *Phys. Rev.* **31**, 579 (1928).

⁴ Condon, *Proc. Nat. Acad. Sci.* **13**, 466 (1927).

⁵ Eisenschitz and London, *Zeits. f. Physik* **60**, 491 (1927).

enough number of parameters, and if one puts in enough labor one can generally approach the right answer, at least as far as the energy is concerned.

However, rather than to do this, it seems preferable to try to get an appreciable improvement in the calculated results with but a small increase in the complexity of the calculation. It is therefore the purpose of the present paper to try to improve the theoretical results for the normal hydrogen molecule, at the same time keeping the wave functions and the calculation as simple as possible.

II. THEORY

To carry out this policy of simplicity, we begin with the understanding that we shall deal only with wave functions made up of products of individual electron wave functions. We then inquire as to what happens to the electron charge distribution in a hydrogen atom when it is brought up to another similar atom so as to combine with it. It is apparent that because of the various complicated interactions that occur, the charge distribution will be altered, this distortion becoming greater as the two atoms approach each other. The wave functions (from which the charge distributions are calculated) also become altered. The exact nature of the changes can be investigated only in a six-dimensional space, but for the purposes of the present problem one can try to consider the approximate distortion of an individual wave function in ordinary space. The simplest way to represent this distortion is to consider the radius of the atom to change with the distance to the other atom. This is effectively what Wang³ did in his calculations, and it led to a definite improvement in the energy value.

However, since the perturbations involved are not spherically symmetrical this cannot be a very good approximation to the true state of affairs, and the next improvement that suggests itself is to introduce a change in the wave function that will depend on the direction with respect to the molecular axis and will be greatest in the direction of the latter. Since the interactions can be thought of roughly as being along this axis, it seems likely that the electron cloud tends to bulge out in the direction of the second atom.

Let us denote the nuclei by a and b , the electrons by 1 and 2, the internuclear distance by R , other distances by r with subscripts and the angle between a radius vector and the axis (the line joining the nuclei) by θ with subscripts. In accordance with the previous considerations we take as the simplest individual wave function

$$\psi = \psi^0 + \sigma\psi' \quad (1)$$

where ψ^0 is the hydrogenic wave function for the lowest state, but with a shielding constant, ψ' is a function symmetrical about the axis but not about a plane through the nucleus perpendicular to it, and σ is a parameter the magnitude of which is to be determined so as to minimize the variational integral.

The conditions imposed on the choice of ψ' are: (1) that it satisfy the boundary conditions for a wave function, (2) that it have reasonable direc-

tional properties, (3) that it be orthogonal to ψ^0 , (4) that it satisfy a simple wave equation. Of these, (1) and (2) are necessary, but (3) and (4) are convenient in calculating. If we consider electron 1 on atom a and write the hydrogenic function in the form

$$\psi^0(a1) = N_0 e^{-\alpha r_{a1}} \quad (2)$$

then the simplest perturbation function satisfying these conditions seems to be

$$\psi'(a1) = N_1 e^{-\alpha r_{a1}} r_{a1} \cos \theta_{a1} \quad (3)$$

where N_0 and N_1 are the corresponding normalizing factors which, on integrating the squares of the wave functions over all space, one finds to have the values:

$$N_0 = (\alpha^3/\pi)^{1/2} \quad (4)$$

$$N_1 = (\alpha^5/\pi)^{1/2}. \quad (5)$$

In these expressions, we have used α to represent the quantity Z/a_0 , where Z is the effective charge of the nucleus and a_0 the normal hydrogen radius. Accordingly, the wave equation satisfied by $\psi^0(a1)$ is

$$H_{a1}^0 \psi^0(a1) = Z^2 E_0 \psi^0(a1) \quad (6)$$

where

$$H_{a1}^0 = -\frac{\hbar^2}{8\pi^2 m} \nabla_1^2 - Ze^2/r_{a1} \quad (7)$$

and E_0 is the energy of a normal hydrogen atom.

Now ψ' can be seen to be identical with the wave function corresponding to the $2p$ state in a hydrogenic atom of nuclear charge $2Z$. Hence the equation which it satisfies is:

$$H_{a1}' \psi'(a1) = Z^2 E_0 \psi'(a1), \quad (8)$$

where

$$H_{a1}' = -\frac{\hbar^2}{8\pi^2 m} \nabla_1^2 - 2Ze^2/r_{a1}. \quad (9)$$

Of course similar expressions can be written for the wave functions for the other electron or atom. Incidentally, it may be mentioned that for the atom b we take for the wave function

$$\psi'(b1) = -N_1 e^{-\alpha r_{b1}} r_{b1} \cos \theta_{b1} \quad (3a)$$

so as to keep all quantities symmetrical about the plane midway between the nuclei.

For the combined wave function of the normal state of the molecule we take

$$\Psi = \psi(a1)\psi(b2) + \psi(b1)\psi(a2). \quad (10)$$

The wave-mechanical Hamiltonian is given by

$$H = -\frac{\hbar^2}{8\pi^2 m} (\nabla_1^2 + \nabla_2^2) + e^2 [1/R - 1/r_{a1} - 1/r_{a2} - 1/r_{b1} - 1/r_{b2} + 1/r_{12}], \quad (11)$$

and according to the theory of the variational method it is necessary to minimize the quantity

$$W = \int \Psi H \Psi dv_1 dv_2 / \int \Psi^2 dv_1 dv_2, \quad (12)$$

which then gives the value of the energy.

Now by making use of Eqs. (6) and (8) we can write

$$H\psi^0(a1)\psi^0(b2) = \{2Z^2E_0 + e^2[1/R + s/r_{a1} + s/r_{b2} - 1/r_{a2} - 1/r_{b1} + 1/r_{12}]\}\psi^0(a1)\psi^0(b2), \quad (13)$$

$$H\psi^0(a1)\psi'(b2) = \{2Z^2E_0 + e^2[1/R + s/r_{a1} + (2s+1)/r_{b2} - 1/r_{a2} - 1/r_{b1} + 1/r_{12}]\}\psi^0(a1)\psi'(b2), \quad (14)$$

$$H\psi'(a1)\psi'(b2) = \{2Z^2E_0 + e^2[1/R + (2s+1)/r_{a1} + (2s+1)/r_{b2} - 1/r_{a2} - 1/r_{b1} + 1/r_{12}]\}\psi'(a1)\psi'(b2), \quad (15)$$

where

$$s = Z - 1. \quad (15a)$$

By means of these relations and similar ones derived from them by replacing a by b or 1 by 2, W can be evaluated. If we adopt the following notation,

$$I_{00} = \int \psi^0(a1)\psi^0(b1)dv_1, \quad (16)$$

$$F_0 = \int \frac{[\psi^0(a1)]^2}{r_{a1}} dv_1, \quad (17)$$

$$G_{00} = \int \frac{[\psi^0(a1)]^2}{r_{b1}} dv_1, \quad (18)$$

$$K_{00,01} = \int \frac{[\psi^0(a1)]^2\psi^0(b2)\psi'(b2)}{r_{12}} dv_1 dv_2, \quad (19)$$

$$J_{01} = \int \frac{\psi^0(a1)\psi'(b1)}{r_{a1}} dv_1; \quad J_{10} = \int \frac{\psi'(a1)\psi^0(b1)}{r_{a1}} dv_1, \quad (20)$$

$$L_{01,10} = \int \frac{\psi^0(a1)\psi'(b1)\psi'(a2)\psi^0(b2)}{r_{12}} dv_1 dv_2, \quad (21)$$

with corresponding changes in the numbering when ψ^0 is replaced by ψ' or vice versa, we can then write W in the form:

$$W = \frac{e^2}{R} \sum_{i=0}^4 \sigma^i (P_i + sQ_i) / \sum_{i=0}^4 \sigma^i D_i + 2Z^2E_0, \quad (22)$$

where the quantities D_i , P_i , and Q_i are made up of the various integrals over wave functions and are defined as follows. In each case the "exchange" terms are grouped in brackets.

$$\left. \begin{aligned} D_0 &= 1 + [I_{00}^2], \\ D_1 &= [4I_{00}I_{01}], \\ D_2 &= 2 + [4I_{01}^2 + 2I_{00}I_{11}], \\ D_3 &= [4I_{01}I_{11}], \\ D_4 &= 1 + [I_{11}^2]. \end{aligned} \right\} (23)$$

$$\left. \begin{aligned} P_0 &= 1 + R(K_{00,00} - 2G_{00}) + [I_{00}^2 + R(L_{00,00} - 2I_{00}J_{00})], \\ P_1 &= 4R(K_{00,01} - G_{01}) + [4I_{00}I_{01} + R(4L_{00,01} - 4I_{01}J_{00} - 2I_{00}J_{01})], \\ P_2 &= 2 + R(4K_{01,01} + 2F_1 + 2K_{00,11} - 2G_{00} - 2G_{11}), \\ &\quad + [4I_{01}^2 + 2I_{00}I_{11} + R(2L_{01,10} + 2L_{01,01} + 2L_{00,11} \\ &\quad - 2I_{11}J_{00} - 4I_{01}J_{01})], \\ P_3 &= 4R(K_{01,11} - G_{01}) + [4I_{01}I_{11} + R(4L_{01,11} - 2I_{11}J_{01})], \\ P_4 &= 1 + R(2F_1 + K_{11,11} - 2G_{11}) + [I_{11}^2 + RL_{11,11}]. \end{aligned} \right\} (24)$$

$$\left. \begin{aligned} Q_0 &= 2RF_0 + [2RI_{00}J_{00}], \\ Q_1 &= [R(4I_{00}J_{10} + 2I_{00}J_{01} + 4I_{01}J_{00})], \\ Q_2 &= R(2F_0 + 4F_1) + [R(4I_{00}J_{11} + 2I_{11}J_{00} + 4I_{01}(J_{01} + 2J_{10}))], \\ Q_3 &= [R(8I_{01}J_{11} + 2I_{11}(J_{01} + 2J_{10}))], \\ Q_4 &= 4RF_1 + [4RI_{11}J_{11}]. \end{aligned} \right\} (25)$$

These integrals can be evaluated without great difficulty. The discussion of them is to be found in the appendix. It is easy to see that the various D_i , P_i , and Q_i are functions only of the quantity

$$\rho = \alpha R \tag{26}$$

and can be calculated for various values of ρ and plotted. If we let

$$\rho_0 = R/a_0, \tag{27}$$

then

$$Z = \rho/\rho_0, \tag{28}$$

$$s = (\rho - \rho_0)/\rho_0. \tag{29}$$

For a given value of R or ρ_0 one can then vary ρ and, by reading the values of the functions from the curves, minimize W . By repeating this for a number of values of ρ_0 one thus obtains a series of energy values which can be plotted as a function of ρ_0 and a smooth curve drawn. However, unless the points for which calculations are made are very close together it is not possible in general to determine the minimum of the energy curve very accurately in this way. If the points are fairly close together one can pass a parabola through the points in the vicinity of the minimum. But if, as was the case in the calculation carried out, the points are not sufficiently close together, one must resort to some other method.

What was done was to use instead of a parabola a curve of the type discussed by Morse⁶ in connection with interatomic potentials:

$$\Delta E = D e^{-2a(\rho_0 - \rho_m)} - 2D e^{-a(\rho_0 - \rho_m)}. \quad (31)$$

A curve of this sort is known to fit molecular energy curves very well especially in the neighborhood of the minimum. By fitting this curve to three points near the minimum one can get the dissociation energy D and the equilibrium distance $\rho_m a_0$. (The details of the curve-fitting are given in the appendix.)

From the latter the moment of inertia follows:

$$J_0 = \frac{1}{2} M_H (\rho_m a_0)^2, \quad (31)$$

where M_H is the mass of a hydrogen atom.

Since at the minimum

$$\frac{d^2 E}{d\rho_0^2} = 2a^2 D \quad (32)$$

the fundamental vibration frequency is given by

$$\nu_0 = \frac{a}{\pi a_0 c} (D/M_H)^{1/2}. \quad (33)$$

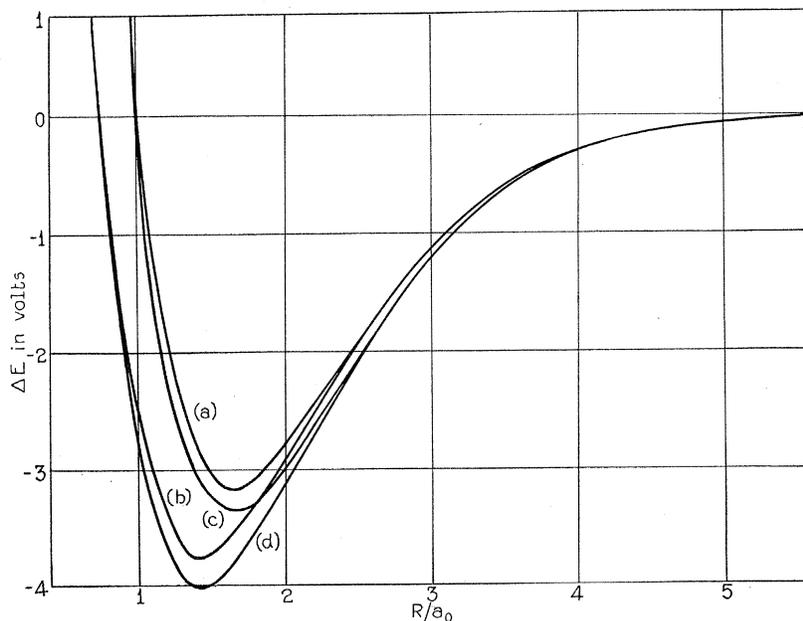


Fig. 1. Calculated energy of normal hydrogen molecule: (a) first order perturbation, (b) varying s , (c) varying σ , (d) varying σ and s .

⁶Morse, Phys. Rev. **34**, 57 (1929).

III. RESULTS

The minimization was carried out first by keeping $\sigma=0$ and varying s . This is essentially what Wang³ did except that his results were only for the equilibrium distance. The energy curve obtained is shown in Fig. 1 (b) and may be compared with the first-order perturbation energy 1 (a).

The value of s as function of the interatomic distance is shown in Fig. 2. For $R=0$ of course we have a helium atom and for this the effective nuclear charge (as given by a variational method calculation) is $1.6875 e$, so that $s = 0.6875$. For large distances s falls off rapidly. It is interesting to note that beyond a certain distance, s changes sign. This may be interpreted by saying that for large distances the second electron has more of an effect upon the atom than the second nucleus. Geometrically one may say that as the atoms

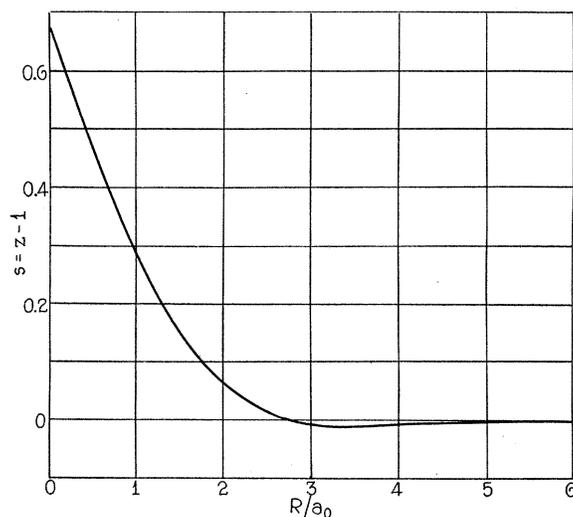


Fig. 2. Variation of s with interatomic distance.

approach each other, there is first an expansion of the charges and then, for smaller distances, a contraction.

The next step in the procedure was to set $s=0$, and minimize W with respect to σ . The energy resulting from this calculation is shown in Fig. 1 (c). Comparison with 1 (a) shows that the improvement in the energy near the equilibrium distance is rather small, but that there is a distinct improvement at somewhat larger distances. The curve of σ thus obtained, denoted by σ_0 , is shown in Fig. 3 (a).

The quantity σ can be taken as a rough measure of the longitudinal distortion of the wave function. As the graph shows, for small distances there seems to be a sudden distortion of the wave function which disappears as the atoms merge to give helium. This apparent behavior at small distances is probably without significance, since the wave functions obtainable from a variational calculation need not approximate the true wave functions as closely as the calculated energy does the true value. In the present case, the

behavior of the true wave functions for small internuclear distance is exceedingly complex, and an attempt to fit this behavior into the narrow mold provided by a single parameter cannot be expected to be very successful.

To get a better approximation, the values of s obtained previously were put into W and then σ was varied once more. The energy obtained this time is given in Fig. 1 as curve (d). As is to be expected, it is below the other curves and merges with (b) for small distances and with (c) for large distances. The curve of the values of σ thus calculated, denoted by σ_1 , is shown in Fig. 3 (b). It agrees with σ_0 down to about $\sigma_0 = 1.5$. For smaller distances the two differ widely, and this is probably the region in which they lose any physical significance they may have at larger distances.

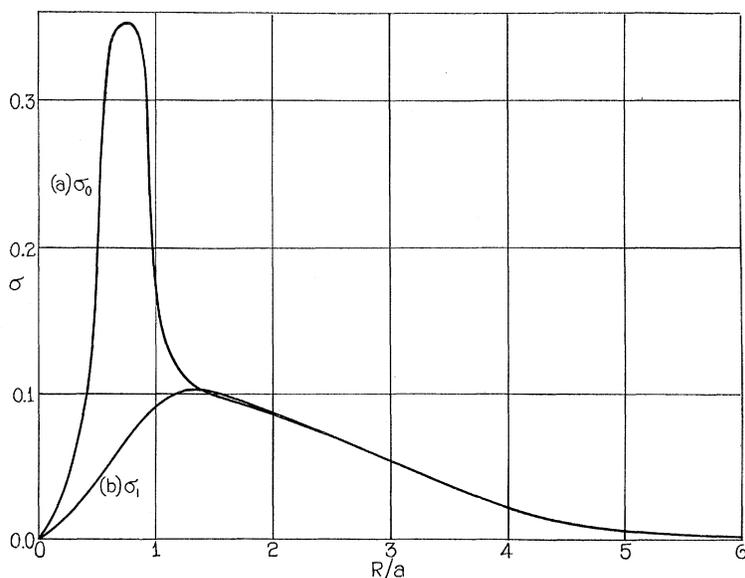


Fig. 3. Parameter σ to minimize energy: (a) without shielding constant, (b) with shielding constant.

The parameter was kept fixed at the set of values σ_1 and s was recalculated. It was found that within the accuracy available in reading graphs, s did not change appreciably—at least in the regions of any importance. Hence the energy curve 1 (d) represents the best result obtainable by the present method.

For this curve the dissociation energy was found to be 4.02 volts, the equilibrium distance between atoms $1.416 a_0$ corresponding to a moment of inertia of 4.66×10^{-41} gm-cm² and a fundamental vibration frequency of 4260 cm⁻¹. In the following table⁷ these results are compared with those obtained in previous calculations and with the experimental values.

⁷ This table (except for obvious changes) is taken from the paper of Wang (reference 3). The experimental values given these are those of Witmer, Proc. Nat. Acad. Sci. **12**, 238 (1926), and Phys. Rev. **28**, 1223 (1926). Cf. Birge, Int. Crit. Table V, 409 (1929).

	E (Rh)	$\Delta E(\psi)$	$J_0(\text{gm}-\text{cm}^2)$	$\nu_0(\text{cm}^{-1})$
Present paper	-2.297	-4.02	4.66×10^{-41}	4260
Wang ³	-2.278	-3.76	4.59	4900
Condon ⁴	-2.325	-4.40	4.26	5300
Sugiura ¹	-2.24	-3.2	5.2	4800
Observed ⁷	-2.326	-4.42	4.67	4380

It is seen that the dissociation energy as calculated here is about 10 per cent too small. However, if we consider the total energy of the molecule, the error is only about 1 per cent. If we compare this to the helium problem—it is only fair that the total molecular energy be considered in this comparison—we note that the Hartree method⁸ gives for the total energy of an He atom 5.75 Rh as compared to 5.81 Rh as observed, so that the error is also about 1 per cent. Now the Hartree method gives the greatest possible accuracy obtainable with wave functions made up of the products of individual wave functions, it being equivalent to a variational method with a function of complete flexibility. Since in the present case the wave function is likewise made up of products of individual wave functions, it is questionable whether one could hope to exceed this accuracy by very much, the situation in the hydrogen molecule being rather similar to that in the helium atom.

In concluding the main part of this paper, the writer wishes to acknowledge the advice and encouragement received from Drs. J. C. Slater and R. M. Langer and the assistance from Dr. S. Ikehara in checking parts of the calculation and in compiling the tables.

Note added in proof (December 4, 1931)—Shortly after the present article had been sent to the publisher, the writer learned of the paper of E. A. Hylleraas, *Zeits. f. Phys.* **71**, 739 (1931) "Über die Elektronenterme des Wasserstoffmolekuls," in which, among other things, he calculates the energy of the lowest state of H_2 in very close agreement with the experimental value. However, it ought to be pointed out that one should not compare the results of the present paper with his results, since he multiplies through his calculated value of the energy by a factor obtained by interpolating between values for $R=0$, and $R=\infty$, to get his final result.

APPENDIX

1. Integrals

Many of the integrals arising in the present calculations are not new. Thus a number are to be found in the papers of Heitler and London,² Sugiura,¹ and Bartlett.⁹ However, for the sake of completeness they will all be given here (in perhaps a different form). All but a few of the integrals present no great difficulties in the evaluation. The ones which do give trouble are the exchange integrals and they can be handled in the following way:

On replacing $1/r_{12}$ by its Neumann expansion in terms of Legendre func-

⁸ Gaunt, *Proc. Camb. Phil. Soc.* **24**, 328 (1928).

⁹ Bartlett, *Phys. Rev.* **37**, 507 (1931).

tions of the elliptic coordinates any one of the exchange integrals arising here can be broken up into a sum of terms of the form $H(m, n, \alpha)$ and $S(m, n, \alpha)$ where

$$H(m, n, \alpha) = \int_1^\infty \lambda_1^m e^{-\alpha\lambda_1} Q_0(\lambda_1) d\lambda_1 \int_1^{\lambda_1} \lambda_2^n e^{-\alpha\lambda_2} d\lambda_2 \quad (A1)$$

$$+ \int_1^\infty \lambda_1^n e^{-\alpha\lambda_1} Q_0(\lambda_1) d\lambda_1 \int_1^{\lambda_1} \lambda_2^m e^{-\alpha\lambda_2} d\lambda_2, \quad (A2)$$

$$S(m, n, \alpha) = \int_1^\infty \lambda_1^m e^{-\alpha\lambda_1} d\lambda_1 \int_1^{\lambda_1} \lambda_2^n e^{-\alpha\lambda_2} d\lambda_2,$$

and

$$Q_0(\lambda) = \frac{1}{2} \ln \frac{\lambda + 1}{\lambda - 1}. \quad (A3)$$

To treat these quantities, use is made of the simpler functions¹⁰

$$A_n(\alpha) = \int_1^\infty \lambda^n e^{-\alpha\lambda} d\lambda, \quad (A4)$$

$$F_n(\alpha) = \int_1^\infty \lambda^n e^{-\alpha\lambda} Q_0(\lambda) d\lambda. \quad (A5)$$

These can be shown to satisfy the following recursion formulae^{8,9}:

$$A_n(\alpha) = \frac{1}{\alpha} [e^{-\alpha} + nA_{n-1}(\alpha)], \quad (A6)$$

$$F_n(\alpha) = F_{n-2}(\alpha) + \frac{1}{\alpha} [nF_{n-1}(\alpha) - (n-2)F_{n-3}(\alpha) - A_{n-2}(\alpha)]. \quad (A7)$$

These, together with the "starting" formulae:

$$A_0(\alpha) = e^{-\alpha}/\alpha, \quad (A8)$$

$$F_0(\alpha) = \frac{1}{2} [(\ln 2 + C)e^{-\alpha}/\alpha - Ei(-2\alpha)e^\alpha/\alpha], \quad (A9)$$

$$F_1(\alpha) = \frac{1}{2} [(\ln 2 + C)e^{-\alpha}(1/\alpha + 1/\alpha^2) - Ei(-2\alpha)e^\alpha(-1/\alpha + 1/\alpha^2)] \quad (A9a)$$

$$C = 0.577216 \dots, \quad (A10)$$

are sufficient to compile tables of these functions. Such tables are included in the present paper¹¹ (Tables I and II).

By using these functions the integrations in (A1) and (A2) can be carried out. Thus on inverting the order of integration it follows readily that:

$$S(m, n, \alpha) = \int_1^\infty \lambda_1^n e^{-\alpha\lambda_1} d\lambda_1 \int_{\lambda_1}^\infty \lambda_2^m e^{-\alpha\lambda_2} d\lambda_2 \quad (A11)$$

¹⁰ Zener and Guillemin, Phys. Rev. **34**, 999 (1929). See also Rosen, Phys. Rev. **38**, 255 (1931).

¹¹ Table I is essentially an enlargement of a table of $A_n(\alpha)$ given in the paper by the present writer mentioned in reference⁸, but corrected for several errors mainly in the 5th and 6th figures. Cf. list of errata at the end of the present paper.

TABLE I. $A_n(\alpha)$.

α	0	1	2	3	4	5	6	7	8	9	10
0.5	1.21306	3.63918	1.57698 · 10 ⁻¹	9.58318 · 10 ⁻¹	7.67868 · 10 ⁻²	7.67989 · 10 ⁻³	9.21599 · 10 ⁻⁴	1.29024 · 10 ⁻⁵	2.06438 · 10 ⁻⁷	3.71589 · 10 ⁻⁸	7.43178 · 10 ⁻⁹
1.0	3.67879 · 10 ⁻¹	7.35759 · 10 ⁻¹	1.83940 · 1	5.88607 · 1	2.39122 · 10	1.19929 · 10 ²	7.19940 · 10 ²	5.03995 · 10 ³	4.03200 · 10 ⁴	3.62880 · 10 ⁵	3.62880 · 10 ⁶
1.5	1.48753	2.47922	4.79317 · 10 ⁻¹	1.10739	3.10178 · 1	1.04880 · 10	4.21009 · 10	1.96620 · 10 ²	1.04879 · 10 ³	6.29287 · 10 ³	4.19526 · 10 ⁴
2.0	6.76676 · 10 ⁻²	1.01501	6.96081 · 10 ⁻²	3.21421 · 10 ⁻¹	7.10510 · 10 ⁻¹	1.84394 · 1	5.59950 · 1	1.96659 · 10	7.87313 · 10	3.54359 · 10 ²	1.77186 · 10 ³
2.5	3.28340	4.59676 · 10 ⁻²	1.63564	1.16364	2.19016	4.70866 · 10 ⁻¹	1.16291	3.28899 · 1	1.05576	3.80402 · 10	1.52193 · 10 ²
3.0	1.65957	2.1276	3.13474	4.79431 · 10 ⁻²	8.05198 · 10 ⁻²	1.50795	3.18186 · 10 ⁻¹	7.59031 · 10 ⁻¹	2.04068 · 1	6.13863 · 1	2.04787 · 10
3.5	8.62782 · 10 ⁻³	1.10929	1.49666	2.14564	3.31494	5.59841 · 10 ⁻²	1.04601	2.17829	5.06522 · 10 ⁻¹	1.31111	3.75467 · 1
4.0	4.57891	5.72364 · 10 ⁻³	7.44073 · 10 ⁻³	1.01595	1.47384	2.30019	3.90871 · 10 ⁻²	7.29719 · 10 ⁻²	1.50523	3.43235 · 10 ⁻¹	8.62716 · 10 ⁻¹
4.5	2.46867	3.01726	3.80967	5.00845 · 10 ⁻³	6.92062 · 10 ⁻³	1.01582	1.60130	2.73778	5.11402 · 10 ⁻²	1.04749	2.35245
5.0	1.34759	1.61711	1.99443	2.54425	3.38299	4.73058 · 10 ⁻³	7.02428 · 10 ⁻³	1.11816	1.92381	3.59762 · 10 ⁻²	7.33000 · 10 ⁻²
6.0	4.13125 · 10 ⁻¹	4.81980 · 10 ⁻¹	5.73785 · 10 ⁻¹	7.00018 · 10 ⁻¹	8.79804 · 10 ⁻¹	1.14630	1.55942	2.23245 · 10 ⁻³	3.38972 · 10 ⁻³	5.49771 · 10 ⁻³	9.57598 · 10 ⁻³
7.0	1.30269	1.48879	1.72806	2.04328	2.47028	3.07409 · 10 ⁻⁴	3.93169 · 10 ⁻⁴	5.23438 · 10 ⁻⁴	7.28484 · 10 ⁻⁴	1.06689	1.65440
8.0	4.19328 · 10 ⁻⁵	4.71744 · 10 ⁻⁵	5.37264 · 10 ⁻⁵	6.20802 · 10 ⁻⁵	7.29729 · 10 ⁻⁵	8.75409 · 10 ⁻⁵	1.07589	1.36073	1.78006	2.42189 · 10 ⁻⁴	3.44669 · 10 ⁻⁴
9.0	1.37122	1.52358	1.70979	1.94115	2.23395	2.61231	3.11276 · 10 ⁻³	3.79225 · 10 ⁻³	4.74211 · 10 ⁻³	6.11333 · 10 ⁻³	8.16381 · 10 ⁻³
10	4.53999 · 10 ⁻⁶	4.99399 · 10 ⁻⁶	5.53879 · 10 ⁻⁶	6.20163 · 10 ⁻⁶	7.02065 · 10 ⁻⁶	8.05032 · 10 ⁻⁶	9.37018 · 10 ⁻⁶	1.10991	1.34193	1.66174	2.11573
12	5.12018 · 10 ⁻⁷	5.54686 · 10 ⁻⁷	6.04465 · 10 ⁻⁷	6.63134 · 10 ⁻⁷	7.33062 · 10 ⁻⁷	8.17460 · 10 ⁻⁷	9.20748 · 10 ⁻⁷	1.04912 · 10 ⁻⁶	1.21143 · 10 ⁻⁶	1.42059 · 10 ⁻⁶	1.69384 · 10 ⁻⁶
14	5.93949 · 10 ⁻⁸	6.36374 · 10 ⁻⁸	6.84860 · 10 ⁻⁸	7.40705 · 10 ⁻⁸	8.05579 · 10 ⁻⁸	8.81656 · 10 ⁻⁸	9.71802 · 10 ⁻⁸	1.07983 · 10 ⁻⁷	1.21101 · 10 ⁻⁷	1.37245 · 10 ⁻⁷	1.57427 · 10 ⁻⁷

TABLE I. $A_n(\alpha)$. (Cont.)

α	11	12	13	14	15	16	17	18	19	20
1.0	3.99168 · 10 ⁷	4.79002 · 10 ⁸	6.22702 · 10 ⁹	8.71783 · 10 ¹⁰	1.30767 · 10 ¹²	2.09228 · 10 ¹³	3.55687 · 10 ¹⁴	6.40237 · 10 ¹⁵	1.21645 · 10 ¹⁷	2.43290 · 10 ¹⁸
2.0	9.74530 · 10 ⁸	5.84719 · 10 ⁴	3.80067 · 10 ⁵	2.66047 · 10 ⁶	1.99539 · 10 ⁷	1.59628 · 10 ⁸	1.35684 · 10 ⁹	1.22116 · 10 ¹⁰	1.16010 · 10 ¹¹	1.16010 · 10 ¹²
3.0	2.37705 · 1	3.00437 · 10 ²	1.30191 · 10 ³	6.07560 · 10 ⁴	3.03780 · 10 ⁵	1.62016 · 10 ⁶	9.18091 · 10 ⁶	5.50835 · 10 ⁶	3.48875 · 10 ⁷	2.32583 · 10 ⁸
4.0	1.62608 · 10 ⁻¹	3.13573 · 1	2.31957 · 10	8.11895 · 10	3.04465 · 10 ²	1.21787 · 10 ³	5.17593 · 10 ³	2.32917 · 10 ⁴	1.06376 · 10 ⁵	5.53178 · 10 ⁵
5.0	1.79691 · 10 ⁻²	3.91606 · 10 ⁻¹	1.01952 · 1	2.85601 · 1	8.56938 · 1	2.74234 · 10	9.32408 · 10	3.35668 · 10 ²	1.27554 · 10 ³	5.10216 · 10 ³
6.0	2.73004 · 10 ⁻³	3.63513 · 10 ⁻²	7.91743 · 10 ⁻²	1.85153 · 10 ⁻¹	4.63296 · 10 ⁻¹	1.23587 · 1	3.50204 · 1	1.05065 · 10	3.32711 · 10	1.10904 · 10 ²
7.0	5.15853 · 10 ⁻⁴	4.81034 · 10 ⁻³	9.06375 · 10 ⁻³	1.82578 · 10 ⁻²	3.92541 · 10 ⁻²	8.98538 · 10 ⁻²	2.18347 · 10 ⁻¹	5.61593 · 10 ⁻¹	1.52445 · 1	4.35572 · 1
8.0	1.13492	8.15712 · 10 ⁻⁴	1.36747	2.43500 · 10 ⁻³	4.60755 · 10 ⁻³	9.25704 · 10 ⁻³	1.97131 · 10 ⁻²	4.43965 · 10 ⁻²	1.05484 · 10 ⁻¹	2.63751 · 10 ⁻¹
9.0	2.78131 · 10 ⁻⁵	1.65035	2.52096 · 10 ⁻⁴	4.05862 · 10 ⁻⁴	6.90148 · 10 ⁻⁴	1.24064	2.35715 · 10 ⁻³	4.72801 · 10 ⁻³	9.99506 · 10 ⁻³	2.22350 · 10 ⁻²
10	2.8151 · 10 ⁻⁶	3.79157 · 10 ⁻⁵	7.99025 · 10 ⁻⁵	1.24394	6.90148 · 10 ⁻⁴	2.03570 · 10 ⁻⁴	3.50609 · 10 ⁻⁴	6.35639 · 10 ⁻⁴	1.21225	2.42904 · 10 ⁻³
12	2.06654 · 10 ⁻⁶	2.57856 · 10 ⁻⁶	3.30546 · 10 ⁻⁶	4.36838 · 10 ⁻⁶	5.97250 · 10 ⁻⁶	8.47535 · 10 ⁻⁶	1.25188 · 10 ⁻⁵	1.92902 · 10 ⁻⁵	3.10548 · 10 ⁻⁵	5.22700 · 10 ⁻⁵
14	1.83088 · 10 ⁻⁷	2.16327 · 10 ⁻⁷	2.60270 · 10 ⁻⁷	3.19665 · 10 ⁻⁷	4.01893 · 10 ⁻⁷	5.18702 · 10 ⁻⁷	6.89247 · 10 ⁻⁷	9.45569 · 10 ⁻⁷	1.34267 · 10 ⁻⁶	1.97949 · 10 ⁻⁶

TABLE II. $F_n(\alpha)$.

α	0	1	2	3	4	5	6	7	8	9	10
0.5	7.11802 · 10 ⁻¹	1.41200	3.93368	1.63121 · 10	9.72429 · 10	7.73476 · 10 ²	7.71272 · 10 ⁸	9.24103 · 10 ⁴	1.29282 · 10 ⁶	2.06747 · 10 ⁷	3.72021 · 10 ⁸
1.0	3.00133	4.67340 · 10 ⁻¹	8.66934 · 10 ⁻¹	2.03225 · 1	6.22186 · 1	2.46547 · 10	1.22109 · 10 ²	7.28378 · 10 ²	5.08127 · 10 ³	4.05651 · 10 ⁴	3.64585 · 10 ⁵
1.5	1.44136	2.01240	3.13287	5.66441 · 10 ⁻¹	1.23593	3.32138 · 1	1.09431 · 10	4.32774 · 10	2.00403 · 10 ²	1.06335 · 10 ³	6.36072 · 10 ³
2.0	7.34145 · 10 ⁻²	9.61588 · 10 ⁻²	1.35740	2.12310	3.79616 · 10 ⁻¹	7.97031 · 10 ⁻¹	1.99083 · 1	5.89394 · 1	2.03758 · 10	8.07840 · 10	3.61354 · 10 ²
2.5	3.86961	4.85789	6.44256 · 10 ⁻²	9.20242 · 10 ⁻²	1.44958	2.58084	5.29515 · 10 ⁻¹	1.26246	3.48483 · 1	1.10096	3.92603 · 10
3.0	2.08628	2.54062	3.22684	4.33445	6.26745 · 10 ⁻²	9.95525 · 10 ⁻²	1.77147	3.58173 · 10 ⁻¹	8.27106 · 10 ⁻¹	2.17314 · 1	6.43555 · 1
3.5	1.14309	1.36042	1.67396	2.13170	2.92805	4.28677	6.87058 · 10 ⁻²	1.22453	2.45229	5.53394 · 10 ⁻¹	1.40174
4.0	6.33936 · 10 ⁻³	7.41008 · 10 ⁻³	8.89967 · 10 ⁻³	1.10691	1.44035	1.98589	4.94382	8.51210 · 10 ⁻²	8.51210 · 10 ⁻²	1.69383	3.75707 · 10 ⁻¹
4.5	3.54908	4.08877	4.81772	5.84140 · 10 ⁻³	7.34625 · 10 ⁻³	9.67909 · 10 ⁻³	1.35214	2.02926	3.31332	5.94416 · 10 ⁻²	1.17786
5.0	2.00209	2.27912	2.64422	3.14181	3.84713	4.89356	6.52936 · 10 ⁻³	9.24142 · 10 ⁻³	1.40385	2.31333	4.16712 · 10 ⁻²
6.0	6.48493 · 10 ⁻⁴	7.24630 · 10 ⁻⁴	8.21182 · 10 ⁻⁴	9.46806 · 10 ⁻⁴	1.11521	1.34889	1.68626	2.19580	3.00521 · 10 ⁻³	4.36423 · 10 ⁻³	6.78624 · 10 ⁻³
7.0	2.13850	2.35680	2.62577	2.96395	3.39922 · 10 ⁻⁴	3.97474 · 10 ⁻⁴	4.75955 · 10 ⁻⁴	5.86811 · 10 ⁻⁴	7.49738 · 10 ⁻⁴	1.00003	1.40364
8.0	7.14706 · 10 ⁻⁵	7.79300 · 10 ⁻⁵	8.57115 · 10 ⁻⁵	9.52412 · 10 ⁻⁵	1.07134	1.22298	1.42115	1.68747	2.05690	2.58789 · 10 ⁻⁴	3.38179 · 10 ⁻⁴
9.0	2.11359	2.60941	2.84110	3.11898	3.45747 · 10 ⁻⁵	3.87708 · 10 ⁻⁵	4.40776 · 10 ⁻⁵	5.09427 · 10 ⁻⁵	6.00541 · 10 ⁻⁵	7.25006 · 10 ⁻⁵	9.00590 · 10 ⁻⁵
10	8.21890 · 10 ⁻⁶	8.82415 · 10 ⁻⁶	9.52973 · 10 ⁻⁶	1.03618	1.13557	1.25606	1.40453	1.59094	1.82994	2.14372	2.56673
12	9.71638 · 10 ⁻⁷	1.03210	1.10099	1.18015 · 10 ⁻⁶	1.27198 · 10 ⁻⁶	1.37963 · 10 ⁻⁶	1.50733 · 10 ⁻⁶	1.66079 · 10 ⁻⁶	1.84798 · 10 ⁻⁶	2.08007 · 10 ⁻⁶	2.37222 · 10 ⁻⁶
14	1.17125 · 10 ⁻⁷	1.23441 · 10 ⁻⁷	1.30517 · 10 ⁻⁷	1.38497 · 10 ⁻⁷	1.47561 · 10 ⁻⁷	1.57939 · 10 ⁻⁷	1.69925 · 10 ⁻⁷	1.83903 · 10 ⁻⁷	2.00383 · 10 ⁻⁷	2.20045 · 10 ⁻⁷	2.43820 · 10 ⁻⁷

TABLE II. $F_n(\alpha)$. (Cont.)

α	11	12	13	14	15	16	17	18	19	20
1.0	3.64239 · 10 ⁶	4.00388 · 10 ⁷	4.80219 · 10 ⁸	6.24040 · 10 ⁹	8.73387 · 10 ¹⁰	1.30976 · 10 ¹²	2.09519 · 10 ¹³	3.56125 · 10 ¹⁴	6.40936 · 10 ¹⁵	1.21764 · 10 ¹⁷
2.0	1.79936 · 10 ³	9.86767 · 10 ³	5.90791 · 10 ⁴	3.83389 · 10 ⁵	2.68033 · 10 ⁶	2.08222 · 10 ⁷	1.60527 · 10 ⁸	1.36357 · 10 ⁹	1.22653 · 10 ¹⁰	1.16466 · 10 ¹¹
3.0	2.12426 · 10	7.73360 · 10	3.07733 · 10 ²	1.32831 · 10 ³	6.18018 · 10 ³	3.08280 · 10 ⁴	1.64105 · 10 ⁵	9.28490 · 10 ⁵	5.56382 · 10 ⁶	3.51998 · 10 ⁷
4.0	9.25241 · 10 ⁻¹	2.51229 · 10	7.46274 · 1	2.40722 · 10	8.37697 · 10	3.12734 · 10 ²	1.24650 · 10 ³	5.28245 · 10 ³	2.37150 · 10 ⁴	1.11425 · 10 ⁵
5.0	8.23454 · 10 ⁻²	1.78373 · 10 ⁻¹	4.21918 · 10 ⁻¹	1.08379 · 1	3.00563 · 1	8.94923 · 1	2.84677 · 10	9.63304 · 10	3.45448 · 10 ²	1.30850 · 10 ³
6.0	1.13816 · 10 ⁻²	2.06797 · 10 ⁻²	4.07512 · 10 ⁻²	8.69442 · 10 ⁻²	2.00110 · 10 ⁻¹	4.94626 · 10 ⁻¹	1.30697 · 1	3.67594 · 1	1.09623 · 10	3.45451 · 10
7.0	2.08938 · 10 ⁻³	3.32048 · 10 ⁻³	5.66027 · 10 ⁻³	1.03720	2.04246 · 10 ⁻²	4.31281 · 10 ⁻²	9.73308 · 10 ⁻²	3.33886 · 10 ⁻¹	5.96233 · 10 ⁻¹	1.60690 · 1
8.0	4.62110 · 10 ⁻⁴	6.64774 · 10 ⁻⁴	1.01289	1.64220 · 10 ⁻³	2.84083 · 10 ⁻³	4.24692 · 10 ⁻³	1.03355	2.16629 · 10 ⁻²	4.81711 · 10 ⁻²	1.13286 · 10 ⁻¹
9.0	1.15726	1.54733	2.16547 · 10 ⁻⁴	3.18946 · 10 ⁻⁴	4.96609 · 10 ⁻⁴	8.19859 · 10 ⁻⁴	1.43697 · 10 ⁻³	2.67310 · 10 ⁻³	5.26965 · 10 ⁻³	1.09841 · 10 ⁻²
10	3.15400 · 10 ⁻⁵	3.99623 · 10 ⁻⁵	5.24757 · 10 ⁻⁵	7.17886 · 10 ⁻⁵	1.02825	2.45950 · 10 ⁻⁴	4.12686 · 10 ⁻⁴	7.13745 · 10 ⁻⁴	1.36990 · 10 ⁻³	3.76551 · 10 ⁻³
12	2.75117 · 10 ⁻⁶	3.24967 · 10 ⁻⁶	3.92398 · 10 ⁻⁶	4.86160 · 10 ⁻⁶	6.20504 · 10 ⁻⁶	8.19299 · 10 ⁻⁶	1.12371 · 10 ⁻⁵	1.60689 · 10 ⁻⁵	2.40296 · 10 ⁻⁵	3.76551 · 10 ⁻⁵
14	2.72997 · 10 ⁻⁷	3.09398 · 10 ⁻⁷	3.55645 · 10 ⁻⁷	4.15593 · 10 ⁻⁷	4.90034 · 10 ⁻⁷	6.02868 · 10 ⁻⁷	7.53104 · 10 ⁻⁷	9.68341 · 10 ⁻⁷	1.28599 · 10 ⁻⁶	1.76966 · 10 ⁻⁶

$$= \frac{m!}{\alpha^{m+1}} \sum_{\nu=0}^m \frac{\alpha^\nu}{\nu!} A_{n+\nu}(2\alpha). \quad (\text{A12})$$

Rather than to calculate $S(m, n, \alpha)$ by this formula it is more convenient when compiling a table of values to use the recursion formula which the expression in A12) satisfies. This is:

$$S(m, n, \alpha) = \frac{1}{\alpha} [mS(m-1, n, \alpha) + A_{m+n}(2\alpha)] \quad (\text{A13})$$

with

$$S(0, n, \alpha) = A_n(2\alpha)/\alpha. \quad (\text{A14})$$

As a check in such calculation, one may use the following relation, easily derivable by the use of expressions of the form (A2) and (A11), namely:

$$S(m, n, \alpha) + S(n, m, \alpha) = A_m(\alpha)A_n(\alpha). \quad (\text{A15})$$

By analogy with (A12) one can define the quantity

$$T(m, n, \alpha) = \frac{m!}{\alpha^{m+1}} \sum_{\nu=0}^m \frac{\alpha^\nu}{\nu!} F_{n+\nu}(2\alpha), \quad (\text{A15})$$

which will have an analogous recursion formula,

$$T(m, n, \alpha) = \frac{1}{\alpha} [mT(m-1, n, \alpha) + F_{m+n}(2\alpha)] \quad (\text{A17})$$

with

$$T(0, n, \alpha) = F_n(2\alpha)/\alpha. \quad (\text{A18})$$

By means of this function, it is found that one can write

$$H(m, n, \alpha) = A_m(\alpha)F_n(\alpha) + A_n(\alpha)F_m(\alpha) - T(m, n, \alpha) - T(n, m, \alpha). \quad (\text{A19})$$

Since the functions (A12), (A18), and (A19) are characterized by three parameters they are too bulky to be tabulated here; however, to calculate them from the tables of $A_n(\alpha)$ and $F_n(\alpha)$ is a simple matter.

By the help of these functions the "exchange" integrals can now be evaluated; the remaining integrals require no special comments. The integrals are as follows:

$$RF_0 = R \int \frac{[\psi^0(a1)]^2}{r_{a1}} dv_1 = \rho \quad (\text{A20})$$

$$RF_1 = R \int \frac{[\psi'(a1)]^2}{r_{a1}} dv_1 = \rho/2 \quad (\text{A21})$$

$$RG_{00} = R \int \frac{[\psi^0(a1)]^2}{r_{b1}} dv_1 = 1 - e^{-2\rho}(\rho + 1) \quad (\text{A22})$$

$$RG_{01} = R \int \frac{\psi^0(a1)\psi'(a1)}{r_{b1}} dv_1 = 1/\rho - e^{-2\rho}(\rho^2 + 2\rho + 2 + 1/\rho) \quad (\text{A23})$$

$$RG_{11} = R \int \frac{[\psi'(a_1)]^2}{r_{b_1}} dv_1 = 1 + 3/\rho^2 - e^{-2\rho}(\rho^3 + 3\rho^2) + 11\rho/2 + 7 + 6/\rho + 3/\rho^2 \quad (A24)$$

$$RK_{00,00} = R \int \frac{[\psi^0(a_1)]^2[\psi^0(b_2)]^2}{r_{12}} dv_1 dv_2 = 1 - e^{-2\rho}(\rho^3/6 + 3\rho^2/4) + 11\rho/8 + 1 \quad (A25)$$

$$RK_{00,01} = R \int \frac{[\psi^0(a_1)]^2\psi^0(b_2)\psi'(b_2)}{r_{12}} dv_1 dv_2 = 1/\rho - e^{-2\rho}(\rho^4/12 + 11\rho^3/24 + 59\rho^2/48 + 2\rho + 2 + 1/\rho) \quad (A26)$$

$$RK_{00,11} = R \int \frac{[\psi^0(a_1)]^2[\psi'(b_2)]^2}{r_{12}} dv_1 dv_2 = 1 + 3/\rho^2 - e^{-2\rho}(\rho^5/20 + 41\rho^4/120 + 301\rho^3/240 + 25\rho^2/8 + 89\rho/16 + 7 + 6/\rho + 3/\rho^2) \quad (A27)$$

$$RK_{01,01} = R \int \frac{\psi^0(a_1)\psi'(a_1)\psi^0(b_2)\psi'(b_2)}{r_{12}} dv_1 dv_2 = 2/\rho^2 - e^{-2\rho}(\rho^5/30 + \rho^4/5 + 77\rho^3/120 + 71\rho^2/48 + 263\rho/96 + 4 + 4/\rho + 2/\rho^2) \quad (A28)$$

$$RK_{01,11} = R \int \frac{\psi^0(a_1)\psi'(a_1)[\psi'(b_2)]^2}{r_{12}} dv_1 dv_2 = 1/\rho + 9/\rho^3 - e^{-2\rho}(\rho^6/60 + 7\rho^5/60 + 113\rho^4/240 + 697\rho^3/480 + 3577\rho^2/960 + 8\rho + 14 + 19/\rho + 18/\rho^2 + 9/\rho^3) \quad (A29)$$

$$RK_{11,11} = R \int \frac{[\psi'(a_1)]^2[\psi'(b_2)]^2}{r_{12}} dv_1 dv_2 = 1 + 6/\rho^2 + 54/\rho^4 - e^{-2\rho}(\rho^7/140 + 141\rho^6/2520 + 19\rho^5/70 + 893\rho^4/840 + 23809\rho^3/6720 + 6411\rho^2/640 + 30731\rho/1280 + 49 + 84/\rho + 114/\rho^2 + 108/\rho^3 + 54/\rho^4) \quad (A30)$$

$$I_{00} = \int \psi^0(a_1)\psi^0(b_1)dv_1 = e^{-\rho}(\rho^2/3 + \rho + 1) \quad (A31)$$

$$I_0 = \int \psi^0(a_1)\psi'(b_1)dv_1 = \rho I_{00}/2 = \frac{1}{2}e^{-\rho}(\rho^3/3 + \rho^2 + \rho) \quad (A32)$$

$$I_{11} = \int \psi'(a_1)\psi'(b_1)dv_1 = e^{-\rho}(\rho^4/15 + 2\rho^3/15 - \rho^2/5 - \rho - 1) \quad (A33)$$

$$RJ_{00} = R \int \frac{\psi^0(a_1)(\psi^0(b_1))}{r_{a_1}} dv_1 = \rho e^{-\rho}(\rho + 1) \quad (A34)$$

$$RJ_{10} = R \int \frac{\psi'(a1)\psi^0(b1)}{r_{a1}} dv_1 = \frac{1}{3}\rho^2 e^{-\rho}(\rho + 1) \quad (\text{A35})$$

$$RJ_{01} = R \int \frac{\psi^0(a1)\psi'(b1)}{r_{a1}} dv_1 = \frac{2}{3}\rho^2 e^{-\rho}(\rho + 1) = 2RJ_{10} \quad (\text{A36})$$

$$RJ_{11} = R \int \frac{\psi'(a1)\psi'(b1)}{r_{a1}} dv_1 = \frac{1}{2}\rho e^{-\rho}(\rho^3/3 - \rho - 1) \quad (\text{A37})$$

$$RL_{00,00} = R \int \frac{\psi^0(a1)\psi^0(b1)\psi^0(a2)\psi^0(b2)}{r_{12}} = (\rho^6/15)[9H(2, 2, \rho) - 6H(2, 0, \rho) + H(0, 0, \rho) - 3S(1, 2, \rho) + S(1, 0, \rho)] \quad (\text{A38})$$

$$RL_{00,01} = R \int \frac{\psi^0(a1)\psi^0(b1)\psi^0(a2)\psi'(b2)}{r_{12}} = (\rho/2)RL_{00,00} \quad (\text{A39})$$

$$R(L_{01,01} + L_{01,10}) = R \int \frac{\psi^0(a1)\psi'(b1)[\psi^0(a2)\psi'(b2) + \psi'(a2)\psi^0(b2)]}{r_{12}} dv_1 dv_2 = (\rho^2/2)RL_{00,00} \quad (\text{A40})$$

$$RL_{00,11} = R \int \frac{\psi^0(a1)\psi^0(b1)\psi'(a2)\psi'(b2)}{r_{12}} dv_1 dv_2 = R \left(\frac{\rho^2}{4} L_{00,00} - L' \right) \quad (\text{A41})$$

$$RL_{01,11} = R \int \frac{\psi^0(a1)\psi'(b1)\psi'(a2)\psi'(b2)}{r_{12}} dv_1 dv_2 = (\rho/2)RL_{00,11} \quad (\text{A42})$$

$$RL_{11,11} = R \int \frac{\psi'(a1)\psi'(b1)\psi'(a2)\psi'(b2)}{r_{12}} dv_1 dv_2 = R \left(\frac{\rho^4}{16} L_{00,00} - \frac{\rho^2}{2} L' + L'' \right). \quad (\text{A43})$$

The primed quantities are given by:

$$RL' = (\rho^8/840)[-21H(6, 2) + 7H(6, 0) + 60H(4, 2) - 20H(4, 0) - 27H(2, 2) + 9H(2, 0) + 21S(5, 2) - 7S(5, 0) - 18S(3, 2) + 6S(3, 0) + 21S(1, 6) - 25S(1, 4) + 6S(1, 2)], \quad (\text{A44})$$

$$RL'' = (\rho^{10}/15120)[147H(6, 6) - 315H(4, 6) + 225H(4, 4) + 63H(2, 6) - 135H(2, 4) + 27H(2, 2) - 294S(5, 6) + 315S(5, 4) - 63S(5, 2) + 217S(3, 6) - 240S(3, 4) + 51S(3, 2)]. \quad (\text{A45})$$

The argument of these functions is ρ as before.

2. Curve Fitting

To fit a curve of the form

$$\Delta E = D e^{-2a(\rho_0 - \rho_m)} - 2D e^{-a(\rho_0 - \rho_m)} \quad (\text{A46})$$

to the energy curve nears its minimum requires a knowledge of the energy at three points in that vicinity. In the calculation discussed the fitting was very easy because the minimum was near $\rho_0 = 1.5$, and values of ΔE had been calculated for $\rho_0 = 1, 1.5, 2$. Thus, if we denote these values of ΔE by E_1, E_2, E_3 , and let

$$B = e^{-a/2}, \quad (\text{A47})$$

$$C = e^{a\rho_m}, \quad (\text{A48})$$

than the equations to be satisfied are:

$$E_1 = CD(CB^4 - 2B^2), \quad (\text{A49})$$

$$E_2 = CD(CB^6 - 2B^3), \quad (\text{A50})$$

$$E_3 = CD(CB^8 - 2B^4). \quad (\text{A51})$$

The solutions are given by the appropriate root of:

$$E_1 B^3 - E_2 B^2 - E_2 B + E_3 = 0, \quad (\text{A52})$$

and by the relations:

$$C = \frac{2}{B^2} \left(\frac{E_1 B - E_2}{E_1 B^2 - E_2} \right), \quad (\text{A53})$$

$$D = \frac{1}{2B^3 C} \left(\frac{E_1 B^2 - E_2}{1 - B} \right), \quad (\text{A54})$$

$$a = 2 \ln(1/B), \quad (\text{A55})$$

$$\rho_m = \frac{1}{a} \ln C. \quad (\text{A56})$$

Thus the constants required in (A46) have been evaluated.

Errata: In a recent paper by the author, *Phys. Rev.* **38**, 255, (1931), several errors appear which may cause inconvenience to anyone using it. The corrected portions should read as follows:

p. 254, Eq. (45): ${}_n^m(\alpha) = \sum_{\nu=0}^m \alpha^\nu F_{n+\nu}(\alpha) / 2^\nu \nu!$

p. 266: $A_8(1, 3.5) = 5.06522$ instead of 5.06553

$A_{10}(1, 3.0) = 2.04787 \cdot 10$ instead of $2.04787 \cdot 1$

$A_{13}(1, 8.0) = 1.36747 \cdot 10^{-3}$ instead of $8.36747 \cdot 10^{-3}$

p. 267: $A_5(-1, 2.0) = 9.23632 \cdot 10^{-1}$ instead of $1.84726 \cdot 10^{-1}$

p. 274, line 5: $\alpha = 1.385 A^{-1}$

p. 274, line 20: 0.87 instead of 1.11.