ORBITAL VALENCY*

By James H. Bartlett, Jr.
Department of Physics, University of Illinois

(Received January 15, 1931)

Abstract

The interaction of two atoms, each with one $2p$ electron, is studied by a method similar to that used by Kemble and Zener. An atomic wave function whose radial part is of the form const. $re^{-kr/2}$ (that is, with no nodes) is used. Complete potential energy curves are obtained for the twelve possible states, which are $^1\Delta_g$, $^3\Delta_u$, $^1\Pi_g$, $^1\Pi_u$, $^3\Pi_g$, $^3\Pi_u$, $^1\Sigma_u^-$, $^3\Sigma_g^-$, two $^1\Sigma_g^+$, and two $^3\Sigma_u^+$. The most stable states are $^3\Sigma_u^+$ (lowest) and $^1\Sigma_g^+$, which arise from $m_{la}=0$ and $m_{lb}=0$, and in which there is the maximum overlapping of charge. The states with least overlapping of charge are those where $m_{la}=\pm 1$ and $m_{lb}=\pm 1$, resulting in $^1\Delta_g$, $^3\Delta_u$, $^1\Sigma_g^+$, $^1\Sigma_u^-$, $^3\Sigma_g^-$, $^3\Sigma_u^+$, which are all repulsive. The Π states lie in between, and are attractive. The present work gives precision to the ideas of Heitler on orbital valency, yields a positive exchange energy integral for the lowest states, and may be taken as supporting the conceptions of Slater about directed valency.

OUR knowledge of the rules underlying the formation of stable diatomic molecules from their constituent atoms is still very limited, in spite of the successes achieved by Heitler and London,[1] and by Kemble and Zener.[2] The idea of spin valency is quite useful, but its general inadequancy has been recognized by Heitler,[3] who has therefore proposed an "orbital" valency. Two atoms can exert on each other forces due not only to the coupling between the spins, but also to the coupling between the orbits, and the two types of interaction may give rise to effects of the same order of magnitude.[4] One must in general take the oribital valency into consideration, and it is highly desirable to formulate rules concerning the order of the resulting molecular states. This is the purpose of the present investigation.

The special problem here studied is that of the interaction of two similar atoms, each with one $2p$ valence electron. For simplicity, a hydrogenic wave function for the atom has been assumed, and the possible influence of internal s electrons has been neglected. Zener[5] has shown that it is legitimate, as an approximation, to assume such a wave function. The method is essentially the same as used by Kemble and Zener,[2] except that in the actual evaluation

* This work was done largely with the aid of a Parker Travelling Fellowship from Harvard University.

[1] W. Heitler u. F. London, Zeits. f. Physik **44**, 455 (1927).

[2] E. C. Kemble and C. Zener, Phys. Rev. **33**, 512 (1929).

[3] W. Heitler, Naturwiss. **17**, 546 (1929).

[4] This statement is rather inexact, but the precise formulation will be made later.

[5] C. Zener, Phys. Rev. **36**, 51 (1930).

of the integrals the procedure of Zener and Guillemin[6] has been followed. Without doubt, one could improve upon the energy values by using a variational method, but it will be assumed that their order would be the same, and it is primarily the order which is the object of this investigation.

We assume, therefore, the radial part of the atomic wave function to be of the form $R = \text{const}\ re^{-\kappa r/2}$, where κ is an arbitrary constant.

Notation. $a(nlm_l/1)$ = wave function for electron 1 on nucleus a, with quantum numbers m, l, m_l. (Similarly for nucleus b).

For one electron, a = distance from nucleus a

b = distance from nucleus b.

For two electrons a_1 = distance of electron one from nucleus a, etc.

R = internuclear distance

r = interelectronic distance

θ_{a1} = angle from internuclear axis to line joining a and 1.

In the case under consideration, it is unnecessary to write explicitly n and l, which are 2 and 1, respectively, for each electron. Accordingly, we shall abbreviate the notation to $a(m_l1)$.

Thus

$$a(11) = c_1 a_1 e^{-\kappa a_1/2} \sin \theta_{a_1} e^{i\phi_1}$$

$$b(02) = c_2 b_2 e^{-\kappa b_2/2} \cos \theta_{b_2}.$$

Kemble and Zener show how one may set up a secular equation for the two-quantum excited states of H_2, and then separate it according to the constants of the motion, the spin-orbit interaction being supposed to be negligible. The same may be done in the present case, and one obtains a secular equation of the twelfth degree, which has eight linear factors, and two quadratic factors. The results are tabulated. The energy is measured from the "unperturbed" value, namely that for infinite separation. $^1\Sigma_g{}^+$ means that the electronic factor of the wave function is unchanged on reflection in a plane through the internuclear axis (+), and on reflection in the midpoint of this axis (g). The notation of Kemble and Zener is also given.

[6] C. Zener and V. Guillemin, Phys. Rev. **34**, 999 (1929).

WAVE FUNCTIONS AND ENERGY LEVELS

m_{la}	m_{lb}	States Symmetry	Wave Function	"Diagonal" Energy
1	1	$^1\Delta_g(S^N)$	$a(11)b(12)+a(12)b(11)$	$\frac{1}{1+S_{11}}(I_1+I_2)$
1	1	$^3\Delta_u(A^N)$	$a(11)b(12)-a(12)b(11)$	$\frac{1}{1-S_{11}}(I_1-I_2)$
1	0	$^1\Pi_g(S^N)$	$a(11)b(02)+a(12)b(01)+a(01)b(12)+a(02)b(11)$	$\frac{1}{1+S_{10}}(I_3+I_4+I_5+I_6)$
1	0	$^1\Pi_u(A^N)$	$a(11)b(02)+a(12)b(01)-a(01)b(12)-a(02)b(11)$	$\frac{1}{1-S_{10}}(I_3-I_4-I_5+I_6)$
1	0	$^3\Pi_g(S^N)$	$a(11)b(02)-a(12)b(01)-a(01)b(12)+a(02)b(11)$	$\frac{1}{1+S_{10}}(I_3+I_4-I_5-I_6)$
1	0	$^3\Pi_u(A^N)$	$a(11)b(02)-a(12)b(01)+a(01)b(12)-a(02)b(11)$	$\frac{1}{1-S_{10}}(I_3-I_4+I_5-I_6)$
1	−1	$^1\Sigma_u^-(A^N)$	$a(11)b(-12)+a(12)b(-11)-a(-11)b(12)-a(-12)b(11)$	$\frac{1}{1-S_{11}}(I_1-I_2-I_7+I_8)$
1	−1	$^3\Sigma_g^-(S^N)$	$a(11)b(-12)-a(12)b(-11)-a(-11)b(12)+a(-12)b(11)$	$\frac{1}{1+S_{11}}(I_1+I_2-I_7-I_8)$
{1	−1	$^1\Sigma_g^+(S^N)$	$a(11)b(-12)+a(12)b(-11)+a(-11)b(12)+a(-12)b(11)$	$\frac{1}{1+S_{11}}(I_1+I_2+I_7+I_8)$
{0	0	$^1\Sigma_g^+(S^N)$	$a(01)b(02)+a(02)b(01)$	$\frac{1}{1+S_{00}}(I_9+I_{10})$
{1	−1	$^3\Sigma_u^+(A^N)$	$a(11)b(-12)-a(12)b(-11)+a(-11)b(12)-a(-12)b(11)$	$\frac{1}{1-S_{11}}(I_1-I_2+I_7-I_8)$
{0	0	$^3\Sigma_u^+(A^N)$	$a(01)b(02)-a(02)b(01)$	$\frac{1}{1-S_{00}}(I_9-I_{10})$

where

$$I_1 = \int H'[a(11)]^2[b(12)]^2 dv$$

$$I_2 = \int H'a(11)b(11)a(12)b(12)dv$$

$$I_3 = \int H'[a(11)]^2[b(02)]^2 dv$$

$$I_4 = \int H'a(11)b(11)a(02)b(02)dv$$

$$I_5 = \int H'a(01)a(11)b(02)b(12)\cos(\phi_1 - \phi_2)dv$$

$$I_6 = \int H'a(11)b(01)a(12)b(02)\cos(\phi_1 - \phi_2)dv$$

$$I_7 = \int H'[a(11)]^2[b(12)]^2 \cos 2(\phi_1 - \phi_2)dv$$

$$I_8 = \int H'a(11)b(11)a(12)b(12) \cos 2(\phi_1 - \phi_2)dv$$

$$I_9 = \int H'[a(01)]^2[b(02)]^2dv$$

$$I_{10} = \int H'a(01)b(01)a(02)b(02)dv$$

$$I_{11} = \int H'a(01)a(12)b(11)b(02) \cos (\phi_1 - \phi_2)dv$$

where H' is the "perturbative" part of the energy, e.g.,

$$H' = \frac{2}{R} + \frac{2}{r} - \frac{2}{a_2} - \frac{2}{b_1}, \text{ using atomic units.}$$

$$(S_{11})^{1/2} = \int a(11)b(11)dv_1, \quad (S_{00})^{1/2} = \int a(01)b(01)dv_1, \quad S_{10} = (S_{11}\ S_{00})^{1/2}.$$

There remain to be solved two two-degree secular equations, namely

$$(1) \qquad \begin{vmatrix} I_1 + I_2 + I_7 + I_8 - E(1 + S_{11}) & 2(I_5 + I_{11}) \\ -I_5 + I_{11} & I_9 + I_{10} - E(1 + S_{00}) \end{vmatrix} = 0$$

and

$$(2) \qquad \begin{vmatrix} I_1 - I_2 + I_7 - I_8 - E(1 - S_{11}) & 2(-I_5 + I_{11}) \\ +I_5 + I_{11} & I_9 - I_{10} - E(1 - S_{00}) \end{vmatrix} = 0$$

The solution of (1) gives us two states of the $^1\Sigma$, S^N type, and the solution of (2) two states of the $^3\Sigma$, A^N type. It turns out that the influence of the non-diagonal terms is negligible.

Evaluation of the Integrals

General formulae. One may classify the integrals according to whether it is necessary to use the Neumann expansion or not in their evaluation. One does not need to do so for the integrals I_1, I_3, I_9, I_5, and I_7. The only term in the Hamiltonian which offers difficulty is the $2/r$ term. The integrals involving the Neumann expansion are termed "exchange," and the others "Coulomb."

Before proceeding, the notation needs explanation. That used by Zener and Guillemin[6] will be adopted.

$$\Gamma_n = \int_0^\infty e^{-u}u^{n-1}du \quad \Gamma_n(\alpha) = \int_\alpha^\infty e^{-u}u^{n-1}du, \quad \gamma_n(\alpha) = \Gamma_n - \Gamma_n(\alpha)$$

$$A_n(\sigma, \alpha) = \int_\sigma^\infty e^{-\alpha x}x^n dx = \frac{1}{\alpha^{n+1}}\Gamma_{n+1}(\sigma\alpha)$$

$$B_n(\alpha) = \int_{-1}^{1} e^{-\alpha x} x^n dx = A_n(-1, \alpha) - A_n(1, \alpha)$$

$$f_\tau(m, \alpha) = \int_{1}^{\infty} e^{-\alpha x} x^m Q_\tau(x) dx$$

where

$$Q_0 = \frac{1}{2} \ln \left(\frac{x+1}{x-1}\right), \quad x > 1, \quad \text{and} \quad Q_1 = xQ_0 - 1.$$

One may readily establish, by partial integration, the following recursion formulae:

$$A_{m+1}(1,\alpha) - A_m(1,\alpha) = \frac{1}{\alpha}\{(m+1)A_m(1,\alpha) - mA_{m-1}(1,\alpha)\}$$

$$A_{m+1}(1,\alpha) + A_m(1,\alpha) = \frac{1}{\alpha}\{2e^{-\alpha} + (m+1)A_m(1,\alpha) + mA_{m-1}(1,\alpha)\}$$

$$A_{m+2}(1,\alpha) - A_m(1,\alpha) = \frac{1}{\alpha}\{(m+2)A_{m+1}(1,\alpha) - mA_{m-1}(1,\alpha)\}$$

$$f_0(n+2,\alpha) - f_0(n,\alpha) = \frac{1}{\alpha}\{-A_n(1,\alpha) + 2f_0(n+1,\alpha) + n[f_0(n+1,\alpha) - f_0(n-1,\alpha)]\}$$

$$f_1(n+2,\alpha) - f_1(n,\alpha) = \frac{1}{\alpha}\{3f_1(n+1,\alpha) - f_0(n,\alpha) + n[f_1(n+1,\alpha) - f_1(n-1,\alpha)]\}$$

$$= \frac{1}{\alpha}\{2f_1(n+1,\alpha) - A_{n-1}(1,\alpha) + (n+1)[f_1(n+1,\alpha) - f_1(n-1,\alpha)]\}$$

We have here used the relations

$$(x^2-1)\frac{dQ_n}{dx} = nxQ_n - nQ_{n-1}, \quad n>0$$

and

$$f_1(m,\alpha) = f_0(m+1,\alpha) - A_m(1,\alpha).$$

Now let

$$F(n, \lambda) = \int_{-1}^{1} \frac{e^{-\rho\mu} d\mu}{(\mu - \lambda)^n}$$

then $F(1) = e^{-\rho\lambda}[-E_i(\rho(1+\lambda)) + E_i(-\rho(1+\lambda))]$ where

$$-E_i(-x) = \int_x^\infty \frac{e^{-u}}{u} du.$$

In general,

$$F(n) = -\frac{1}{n-1}\left[\frac{e^{-\rho}}{(1-\lambda)^{n-1}} - \frac{e^{\rho}}{(-1-\lambda)^{n-1}}\right] - \frac{\rho}{n-1}F(n-1), n \neq 1$$

and

$$\frac{dF(n)}{d\lambda} = nF(n+1).$$

Abbreviating,

$$F_1(n) = -\frac{1}{n-1}\left[\frac{e^{-\rho}}{(1-\lambda)^{n-1}} - \frac{e^{\rho}}{(-1-\lambda)^{n-1}}\right]$$

and

$$F(n) = -\frac{\rho}{n-1}F(n-1) + F_1(n)$$

$$\int_1^\infty f(\lambda)F(n+1)e^{-\rho\lambda}d\lambda = \int_1^\infty f(\lambda)\,\frac{1}{n}\,\frac{dF(n)}{d\lambda}e^{-\rho\lambda}d\lambda = \frac{1}{2n}f(\lambda)F(n)e^{-\rho\lambda}\Big|_1^\infty$$

$$-\frac{1}{2n}\int_1^\infty e^{-\rho\lambda}\left\{F(n)\frac{df(\lambda)}{d\lambda} - f(\lambda)\frac{dF_1(n)}{d\lambda}\right\}d\lambda. \qquad (3)$$

For the most part, two kinds of coordinate systems have been employed. One, with a, b, and ϕ as coordinates, and $(1/R)adabdbd\phi$ as volume element, is most convenient for integrals such as $\int e^{-\kappa a}f(a, b)dv$, since one can integrate over b first and avoid the occurrence of integral logarithms in the final integrand (using a wave function with radial part $R = cre^{-\kappa r/2}$). The other, with λ, μ, and ϕ as coordinates, where $a = (R/2)(\lambda+\mu)$ and $b = (R/2)(\lambda-\mu)$, and $(R/2)^3(\lambda^2-\mu^2)d\lambda d\mu d\phi$ is the volume element, is best for integrals such as $\int e^{-\kappa(a+b)}f(a, b)dv$, the integration over μ being performed first. The transformation is as follows:

$$\cos\theta_a = \frac{\lambda\mu+1}{\lambda+\mu} \quad \cos\theta_b = \frac{\lambda\mu-1}{\lambda-\mu} \quad \sin^2\theta_a = \frac{(\lambda^2-1)(1-\mu^2)}{(\lambda+\mu)^2},$$

$$\sin^2\theta_b = \frac{(\lambda^2-1)(1-\mu^2)}{(\lambda-\mu)^2}.$$

Normalization. The normalized atomic wave functions are $u = c_1e^{-\kappa r/2}r \sin\theta e^{\pm i\phi}$ and $u = c_2e^{-\kappa r/2}\, r\cos\theta$, where $2\pi c_1^2/\kappa^5 = 1/32$ and $2\pi c_2^2/\kappa^5 = 1/16$. Let $\alpha = \kappa R$.

$$(S_{11})^{1/2} = 2\pi c_1^2\int e^{-(\kappa/2)(a+b)}a\sin\theta_a\; b\sin\theta_b\; adabdb$$

$$= \frac{2\pi c_1^2}{\kappa^5}\left(\frac{\alpha}{2}\right)^5\int_1^\infty d\lambda\int_{-1}^1 d\mu e^{-\alpha\lambda/2}(\lambda^2-1)(\lambda^2-\mu^2)(1-\mu^2)$$

$$= 1/24\cdot(\alpha/2)^5\{A_4(1, \alpha/2) - (6/5)A_2(1, \alpha/2) + (1/5)A_0(1, \alpha/2)\}$$

$$(S_{00})^{1/2} = (2\pi c_2^2/\kappa^5)(\alpha/2)^5\int_1^\infty d\lambda\int_{-1}^1 d\mu e^{-\alpha\lambda/2}(\lambda^2\mu^2-1)(\lambda^2-\mu^2)$$

$$= 1/24\cdot(\alpha/2)^5\{A_4(1, \alpha/2) - (18/5)A_2(1, \alpha/2) + A_0(1, \alpha/2)$$

The integrals I_1, I_3, I_9, I_5, I_7.

Let

$$i_1 = \int \frac{2}{r}[a(11)]^2[b(12)]^2 dv = \int \frac{2}{r} c_1^4 a_1^2 b_2^2 \sin^2\theta_{a_1} \sin^2\theta_{b_2} e^{-\kappa(a_1+b_2)} dv$$

$$i_3 = \int \frac{2}{r}[a(11)]^2[b(02)]^2 dv = \int \frac{2}{r} c_1^2 c_2^2 a_1^2 b_2^2 \sin^2\theta_{a_1} \cos^2\theta_{b_2} e^{-\kappa(a_1+b_2)} dv$$

$$= \int \frac{2}{r}[a(01)]^2[b(12)]^2 dv = \int \frac{2}{r} c_1^2 c_2^2 a_1^2 b_2^2 \cos^2\theta_{a_1} \sin^2\theta_{b_2} e^{-\kappa(a_1+b_2)} dv$$

$$i_9 = \int \frac{2}{r}[a(01)]^2[b(02)]^2 dv = \int \frac{2}{r} c_2^4 a_1^2 b_2^2 \cos^2\theta_{a_1} \cos^2\theta_{b_2} e^{-\kappa(a_1+b_2)} dv$$

$$i_5 = \int \frac{2}{r} a(01)a(11)b(02)b(12) \cos(\phi_1 - \phi_2) dv$$

$$= \int \frac{2}{r} c_1^2 c_2^2 a_1^2 b_2^2 \sin\theta_{a_1} \cos\theta_{a_1} \sin\theta_{b_2} \cos\theta_{b_2} e^{-\kappa(a_1+b_2)} \cos(\phi_1 - \phi_2) dv$$

$$i_7 = \int \frac{2}{r}[a(11)]^2[b(12)]^2 \cos 2(\phi_1 - \phi_2) dv$$

$$= \int \frac{2}{r} c_1^4 a_1^2 b_2^2 \sin^2\theta_{a_1} \sin^2\theta_{b_2} e^{-\kappa(a_1+b_2)} \cos 2(\phi_1 - \phi_2) dv.$$

We can now expand $2/r$ as usual:—

$$\frac{2}{r} = \frac{2}{b_1}\left\{1 + \frac{b_2}{b_1}\cos\gamma + \left(\frac{b_2}{b_1}\right)^2 P_2(\cos\gamma) + \cdots\right\} \quad b_2 < b_1$$

$$= \frac{2}{b_2}\left\{1 + \frac{b_1}{b_2}\cos\gamma + \left(\frac{b_1}{b_2}\right)^2 P_2(\cos\gamma) + \cdots\right\} \quad b_2 > b_1$$

where γ is the angle between the lines b_1 and b_2, and

$$P_n(\cos\gamma) = P_n(\cos\theta_{b_1})P_n(\cos\theta_{b_2}) + 2\sum_{m=1}^{n}(-1)^m \frac{(n-m)!}{(n+m)!} P_n{}^m(\cos\theta_{b_1})P_n{}^m(\cos\theta_{b_2}) \cos m(\phi_1 - \phi_2)$$

$$\int_0^{2\pi} P_n(\cos\gamma) \cos m(\phi_1 - \phi_2) d(\phi_1 - \phi_2) = 2\pi P_n(\cos\theta_{b_1})P_n(\cos\theta_{b_2}), \quad m = 0$$

$$= 2\pi(-1)^m \frac{(n-m)!}{(n+m)!} P_n{}^m(\cos\theta_{b_1})P_n{}^m(\cos\theta_{b_2}), \quad m \neq 0.$$

On performing the integrations, one obtains, letting

$$g_{5,1} = \frac{\gamma_5(\kappa b)}{\kappa b} + \Gamma_4(\kappa b)$$

$$g_{7,3} = \frac{\gamma_7(\kappa b)}{(\kappa b)^3} + (\kappa b)^2\Gamma_2(\kappa b),$$

the following expressions:—

$$i_1 = (16\pi c_1^4/3\kappa^4)\int a^2\sin^2\theta_a e^{-\kappa a}[g_{5,1} - (1/5)P_2(\cos\theta_b)g_{7,3}]dv$$

$$i_3 = (8\pi c_1^2 c_2^2/3\kappa^4)\int a^2\sin^2\theta_a e^{-\kappa a}[g_{5,1} + (2/5)P_2(\cos\theta_b)g_{7,3}]dv$$

$$= (16\pi c_1^2 c_2^2/3\kappa^4)\int a^2\cos^2\theta_a e^{-\kappa a}[g_{5,1} - (1/5)P_2(\cos\theta_b)g_{7,3}]dv$$

$$i_9 = (8\pi c_2^4/3\kappa^4)\int a^2\cos^2\theta_a e^{-\kappa a}[g_{5,1} + (2/5)P_2(\cos\theta_b)g_{7,3}]dv$$

$$i_5 = -\ (8\pi c_1^2 c_2^2/5\kappa^4)\int a^2\sin\theta_a\cos\theta_a\sin\theta_b\cos\theta_b e^{-\kappa a}g_{7,3}dv$$

$$i_7 = -\ (8\pi c_1^4/5\kappa^4)\int a^2\sin^2\theta_a\sin^2\theta_b e^{-\kappa a}g_{7,3}dv$$

$$\int a^2\sin^2\theta_a e^{-\kappa a}(\Gamma_5/\kappa b)dv = (8\pi\Gamma_5/3\kappa^5)[g_{5,1}(\alpha) - (1/5)g_{7,3}(\alpha)]$$

$$\int a^2\cos^2\theta_a e^{-\kappa a}(\Gamma_5/\kappa b)dv = (4\pi\Gamma_5/3\kappa^5)[g_{5,1}(\alpha) + (2/5)g_{7,3}(\alpha)]$$

$$\int a^2\sin^2\theta_a e^{-\kappa(a+b)}[(\kappa b)^3 + 6(\kappa b)^2 + 18\kappa b + 24](1/\kappa b)\cdot dv$$

$$= (2\pi/\kappa^5)(\alpha/2)^4\{(\alpha/2)^3[(4/3)(A_6 - A_4) - (4/35)(A_2 - A_0)]$$
$$+ 6(\alpha/2)^2[(4/3)(A_5 - A_3) - (4/15)(A_3 - A_1)] + 18(\alpha/2)[(4/3)(A_4 - A_2)$$
$$- (4/15)(A_2 - A_0)] + 24(4/3)(A_3 - A_1)\}$$

$$\int a^2\cos^2\theta_a e^{-\kappa(a+b)}[(\kappa b)^3 + 6(\kappa b)^2 + 18\kappa b + 24](1/\kappa b)\cdot dv$$

$$= (2\pi/\kappa^5)(\alpha/2)^4\{(\alpha/2)^3[(2/3)(A_6 - A_4) + (46/35)A_2 - (2/5)A_0]$$
$$+ 6(\alpha/2)^2[(2/3)A_5 + (4/15)A_3 + (2/15)A_1] + 18(\alpha/2)[(2/3)A_4 + (8/5)A_2$$
$$- (2/3)A_0] + 24[(2/3)A_3 + (10/3)A_1]\}$$

$$\Gamma_7\int a^2\sin^2\theta_a e^{-\kappa a}P_2(\cos\theta_b)(1/\kappa b)^3 dv$$
$$= (8\pi\Gamma_7/\kappa^5)[\gamma_5/3\alpha^3 - \Gamma_2/15 - 2\gamma_7/5\alpha^5]$$

$$\Gamma_7\int a^2\cos^2\theta_a e^{-\kappa a}P_2(\cos\theta_b)(1/\kappa b)^3 dv$$
$$= (4\pi\Gamma_7/\kappa^5)[\gamma_5/3\alpha^3 + 2\Gamma_2/15 + 4\gamma_7/5\alpha^3 - \alpha^2 e^{-\alpha}/2]$$

$$\int a^2 \sin^2 \theta_a e^{-\kappa a}(1/\kappa b)^3 P_2(\cos\theta_b)[\Gamma_7(\kappa b) - (\kappa b)^5\ \Gamma_2(\kappa b)]dv$$

$$= (2\pi\alpha^2/4\kappa^5)[(\alpha/2)^5\{-(4/3)(A_6 - A_4) + (64/7)(A_4 - A_2) - (12/7)(A_2 - A_0)\}$$
$$+ (\alpha/2)^4\{-8(A_5 - A_3) + 40(A_3 - A_1)\}$$
$$+ 15\alpha^3\{2(A_6 - A_4) - (76/15)(A_4 - A_2) + (62/15)(A_2 - A_0)\}$$
$$+ 90\alpha^2\{-8(A_5 - A_3) + (34/3)(A_3 - A_1)\}$$
$$+ 360\alpha\{(15/2)A_4 - (71/6)A_2 + (10/3)A_0\}]$$

$$\int a^2 \cos^2 \theta_a e^{-\kappa a}(1/\kappa b)^3 P_2(\cos\theta_b)[\Gamma_7(\kappa b) - (\kappa b)^5\ \Gamma_2(\kappa b)]dv$$
$$= (2\pi\alpha^2/4\kappa^5)[(\alpha/2)^5\{(4/3)A_6 - (220/21)A_4 + (124/7)A_2 - 4A_0\}$$
$$+ (\alpha/2)^4\{8A_5 - 64A_3 + 88A_1\}$$
$$+ 15\alpha^3\{-2A_6 - (14/15)A_4 + (6/5)A_2 + (10/3)A_0\}$$
$$+ 90\alpha^2\{8A_5 + (14/3)A_3 - (26/3)A_1\}$$
$$+ 360\alpha\{-(23/2)A_4 - (25/6)A_2 + 2A_0)\}$$
$$+ 720\{8A_3 + 2A_1\}]$$

$$\int a^2 \sin^2 \theta_a e^{-\kappa a}(1/\kappa b)^3[\Gamma_7(\kappa b) - (\kappa b)^5\ \Gamma_2(\kappa b)]dv$$
$$= (2\pi\alpha^2/4\kappa^5)[5(\alpha/2)^5\{(4/3)(A_6 - A_4) - (4/35)(A_2 - A_0)\}$$
$$+ 30(\alpha/2)^4\{(4/3)(A_5 - A_3) - (4/15)(A_3 - A_1)\}$$
$$+ 15\alpha^3\{(4/3)(A_4 - A_2) - (4/15)(A_2 - A_0)\}$$
$$+ 120\alpha^2(A_3 - A_1) + 960(A_2 - A_0)]$$

$$\Gamma_7 \int a^2 \sin\theta_a \cos\theta_a \sin\theta_b \cos\theta_b e^{-\kappa a}(1/\kappa b)^3 dv$$
$$= (2\pi\Gamma_7/15\kappa^5\alpha^3)[-16\gamma_7(\alpha)/\alpha^2 + 4\alpha^3\Gamma_2(\alpha)]$$

$$\int a^2 \sin\theta_a \cos\theta_a \sin\theta_b \cos\theta_b e^{-\kappa a}(1/\kappa b)^3[\Gamma_7(\kappa b) - (\kappa b)^5\ \Gamma_2(\kappa b)]dv$$
$$= (2\pi\alpha^2/4\kappa^5)[(\alpha/2)^5\{(4/3)(A_6 - A_4) - (152/21)(A_4 - A_2) + (1/15)(A_2 - A_0)\}$$
$$+ (\alpha/2)^4\{8(A_5 - A_3) - 40(A_3 - A_1)\}$$
$$+ 20\alpha^3\{(A_6 - A_4) - (1/5)(A_4 - A_2) - 2(A_2 - A_0)\}$$
$$- 480\alpha^2(A_5 - A_3) + 360\alpha\{(23/3)A_4 - 5A_2 - 2A_0\} - 240\{16A_3 - 8A_1\}]$$

Evaluation of the integral

$$\int a^2 \cos^2 \theta_a e^{-\kappa a} P_2(\cos\theta_b)(1/\kappa b)^3 dv = J$$

This is a conditionally convergent integral,[7] the value of which depends upon the particular coordinate system used. Since the companion integral has been evaluated in the λ, μ system (merely for convenience), this procedure must be followed here, even though much more laborious than the evaluation in the a, b, system. Setting $\rho=\alpha/2$,

$$J = \int\int e^{-\alpha(\lambda+\mu)/2}(2\pi/\kappa^5)(\alpha/2)^2(\lambda\mu+1)^2(1/(\lambda-\mu)^3)(\lambda^2-\mu^2)$$

$$\{1-3(\lambda^2-1)(1-\mu^2)/2(\lambda-\mu)^2\}d\lambda d\mu$$

$$= (2\pi\alpha^2/4\kappa^5)\Big[\int\int e^{-\rho(\lambda+\mu)}(\lambda\mu+1)^2(\lambda+\mu)/(\lambda-\mu)^2\cdot d\lambda d\mu$$

$$-(3/2)\int\int(\lambda^2-1)e^{-\rho(\lambda+\mu)}(\lambda\mu+1)^2\{(1-\lambda^2)(\lambda+\mu)/(\lambda-\mu)^4$$

$$+(\lambda+\mu)^2/(\lambda-\mu)^3\}d\lambda d\mu\Big]$$

$$= (2\pi\alpha^2/4\kappa^5)\int_1^\infty e^{-\rho\lambda}d\lambda\left[I_0-(3/2)(\lambda^2-1)\{(1-\lambda^2)I_1+I_2\}\right]$$

where

$$I_0 = \int_{-1}^1 d\mu e^{-\rho\mu}(\lambda\mu+1)^2(\lambda+\mu)/(\lambda-\mu)^2$$

$$I_1 = \int_{-1}^1 d\mu e^{-\rho\mu}(\lambda\mu+1)^2(\lambda+\mu)/(\lambda-\mu)^4$$

$$I_2 = \int_{-1}^1 d\mu e^{-\rho\mu}(\lambda\mu+1)^2(\lambda+\mu)^2/(\lambda-\mu)^3$$

$$I_0 = 2\lambda\{\lambda^2F(0)+2\lambda(\lambda^2+1)F(1)+(\lambda^2+1)^2F(2)\}+\lambda^2F(-1)$$
$$+2\lambda(\lambda^2+1)F(0)+(\lambda^2+1)^2F(1)$$

$$I_1 = 2\lambda\{\lambda^2F(2)+2\lambda(\lambda^2+1)F(3)+(\lambda^2+1)^2F(4)\}+\lambda^2F(1)$$
$$+2\lambda(\lambda^2+1)F(2)+(\lambda^2+1)^2F(3)$$

$$I_2 = -4\lambda^2\{\lambda^2F(1)+2\lambda(\lambda^2+1)F(2)+(\lambda^2+1)^2F(3)\}-4\lambda\{\lambda^2F(0)$$
$$+2\lambda(\lambda^2+1)F(1)+(\lambda^2+1)^2F(2)\}-\{\lambda^2F(-1)+2\lambda(\lambda^2+1)F(0)$$
$$+(\lambda^2+1)^2F(1)\}$$

$$J = (2\pi\alpha^2/4\kappa^5)\int_1^\infty e^{-\rho\lambda}d\lambda\{3\lambda(1-\lambda^4)^2F(4)+(3/2)(1-\lambda^4)(1-9\lambda^4)F(3)$$
$$+(24\lambda^7-\lambda^5-14\lambda^3-\lambda)F(2)+(21\lambda^6-5\lambda^4/2-6\lambda^2-1/2)F(1)$$
$$+(9\lambda^5-2\lambda^3-\lambda)F(0)+(3\lambda^4/2-\lambda^2/2)F(-1)\},$$

[7] This was not realized at first, and the a, b coordinate system was used. This gave a wrong result, and I wish to thank Mr. H. M. Mott-Smith, Jr. for his kindness in helping to locate the error.

Applying formula (3), one obtains

$$J = (4\pi/\kappa^5)(\gamma_5/3\alpha^3 + 2\Gamma_2/15 + 4\gamma_7/5\alpha^5 - \alpha^2 e^{-\alpha}/2).$$

This differs from the result using the a, b coordinate system in that the last term here does not occur in that result.

The integrals i_2, i_4, i_6, i_8, i_{10}, and i_{11}.

$$i_2 = c_1^4 \int dv_1 dv_2 a_1 \sin\theta_{a_1} b_1 \sin\theta_{b_1} a_2 \sin\theta_{a_2} b_2 \sin\theta_{b_2} e^{-(\kappa/2)(a_1+a_2+b_1+b_2)}(2/r)$$

$$i_4 = c_1^2 c_2^2 \int dv_1 dv_2 a_1 \sin\theta_{a_1} b_1 \sin\theta_{b_1} a_2 \cos\theta_{a_2} b_2 \cos\theta_{b_2} e^{-(\kappa/2)(a_1+a_2+b_1+b_2)}(2/r)$$

$$i_6 = c_1^2 c_2^2 \int dv_1 dv_2 a_1 \sin\theta_{a_1} b_1 \cos\theta_{b_1} a_2 \sin\theta_{a_2} b_2 \cos\theta_{b_2} \cos(\phi_1 - \phi_2) e^{-(\kappa/2)(a_1+a_2+b_1+b_2)}(2/r)$$

$$i_8 = c_1^4 \int dv_1 dv_2 a_1 \sin\theta_{a_1} b_1 \sin\theta_{b_1} a_2 \sin\theta_{a_2} b_2 \sin\theta_{b_2} \cos 2(\phi_1 - \phi_2) e^{-(\kappa/2)(a_1+a_2+b_1+b_2)}(2/r)$$

$$i_{10} = c_2^4 \int dv_1 dv_2 a_1 \cos\theta_{a_1} b_1 \cos\theta_{b_1} a_2 \cos\theta_{a_2} b_2 \cos\theta_{b_2} e^{-(\kappa/2)(a_1+a_2+b_1+b_2)}(2/r)$$

$$i_{11} = c_1^2 c_2^2 \int dv_1 dv_2 a_1 \cos\theta_{a_1} b_1 \sin\theta_{b_1} a_2 \sin\theta_{a_2} b_2 \cos\theta_{b_2} \cos(\phi_1 - \phi_2) e^{-(\kappa/2)(a_1+a_2+b_1+b_2)}(2/r).$$

We use Neumann's expansion:

$$\frac{1}{r} = \frac{2}{R} \sum_{\tau=0}^{\infty} \sum_{\nu=0}^{\tau} D_{\tau\nu} P_\tau^\nu \begin{pmatrix}\lambda_1\\ \lambda_2\end{pmatrix} Q_\tau^\nu \begin{pmatrix}\lambda_2\\ \lambda_1\end{pmatrix} P_\tau^\nu(\mu_1) P_\tau^\nu(\mu_2) \cos\nu(\phi_1 - \phi_2)$$

the upper arguments for $\lambda_2 > \lambda_1$, and the lower for $\lambda_2 < \lambda_1$

$$D_{\tau\nu} = (-1)^\nu \epsilon_\nu (2\tau + 1) \left[\frac{(\tau - \nu)!}{(\tau + \nu)!}\right]^2, \quad \epsilon_0 = 1, \ \epsilon_1 = \epsilon_2 = \cdots = 2.$$

One does not need to concern oneself as to whether the above series converges rapidly or not (for the integrals in question), for orthogonality relations reduce the number of terms to three or four. In general, but not always, the second term is so small compared with the first that its contribution may be neglected.

Let us denote the terms arising from $\tau = 0$ by $i_2^{(0)}$, $i_4^{(0)}$, etc. Also, let

$$\sigma_\tau(m, n, \alpha) = \int_1^\infty Q_\tau(\lambda) e^{-\alpha\lambda/2} \lambda^m A_n\left(\lambda, \frac{\alpha}{2}\right) d\lambda$$

$$= \sum_{\nu=0}^{n} (n!/\nu!) f_\tau(m + \nu, \alpha)(\alpha/2)^{\nu-n-1}$$

$$s_\tau(m, n, \alpha) = \int_1^\infty Q_\tau(\lambda_1) e^{-\alpha\lambda_1/2} \lambda_1^m d\lambda_1 \int_1^{\lambda_1} e^{-\alpha\lambda_2/2} \lambda_2^n d\lambda_2$$

$$= f_\tau(m, \alpha/2)\, A_n(1, \alpha/2) - \sigma_\tau(m, n, \alpha)$$

Tables of σ_τ, s_τ, etc. are given later.

$$i_2^{(0)} = 2c_1^4(2\pi)^2(R/2)^9 \int (\lambda_1^2 - 1)(1 - \mu_1)^2(\lambda_2^2 - 1)(1 - \mu_2^2)(\lambda_1^2 - \mu_1^2)$$

$$(\lambda_2^2 - \mu_2^2)Q_0\binom{\lambda_2}{\lambda_1} e^{-\kappa R(\lambda_1+\lambda_2)/2} d\mu_1 d\mu_2 d\lambda_1 d\lambda_2$$

$$= (2\kappa/1024)(\alpha/2)^9 \int (\lambda_1^2 - 1)(\lambda_2^2 - 1)(4/3)^2(\lambda_1^2 - 1/5)$$

$$(\lambda_2^2 - 1/5)Q_0\binom{\lambda_2}{\lambda_1} e^{-\kappa R(\lambda_1+\lambda_2)/2} d\lambda_1 d\lambda_2$$

$$= (\kappa/144)(\alpha/2)^9\{s_0(00)/25 + 36s_0(22)/25 + s_0(44) - 6[s_0(02) + s_0(20)]/25 + [s_0(04) + s_0(40)]/5 - 6[s_0(24) + s_0(42)]/5\}$$

$$i_4^{(0)} = (\kappa/144)(\alpha/2)^9\{s_0(00)/5 + 108s_0(22)/25 + s_0(44) - 24[s_0(02) + s_0(20)]/25 + 3[s_0(04) + s_0(40)]/5 - 12[s_0(42) + s_0(24)]/5\}$$

$$i_{10}^{(0)} = (\kappa/16)(\alpha/2)^9[\{s_0(00) + s_0(04) + s_0(40) + s_0(44)\}/9 + 36s_0(22)/25 - 2\{s_0(02) + s_0(20) + s_0(42) + s_0(24)\}/5]$$

Let

$$t_2(2m, 2n, \alpha) = \int_1^\infty Q_2(\lambda_1)e^{-\alpha\lambda_1/2}\lambda_1^{2m}d\lambda_1 \int_1^{\lambda_1} P_2(\lambda_2)e^{-\alpha\lambda_2/2}\lambda_2^{2n}d\lambda_2$$

$$= (3/2)s_2(2m, 2n + 2) - (\tfrac{1}{2})s_2(2m, 2n).$$

Then

$$i_2^{(2)} = 10c_1^4(2\pi)^2(R/2)^9 \int(\lambda_1^2 - 1)(1 - \mu_1)^2(\lambda_2^2 - 1)(1 - \mu_2^2)(\lambda_1^2 - \mu_1^2)$$

$$(\lambda_2^2 - \mu_2^2)e^{-\alpha(\lambda_1+\lambda_2)/2}\cdot Q_2\binom{\lambda_2}{\lambda_1} P_2\binom{\lambda_1}{\lambda_2} P_2(\mu_1)P_2(\mu_2)d\mu_1 d\mu_2 d\lambda_1 d\lambda_2$$

$$= 10c_1^4(2\pi)^2(R/2)^9 \int (4/15)^2(\lambda_1^2 - 1)(\lambda_2^2 - 1)(\lambda_1^2 + 1/7)$$

$$(\lambda_2^2 + 1/7)Q_2\binom{\lambda_2}{\lambda_1} P_2\binom{\lambda_1}{\lambda_2} e^{-\alpha(\lambda_1+\lambda_2)/2} d\lambda_1 d\lambda_2$$

$$= (\kappa/720)(\alpha/2)^9[t_2(00)/49 + 36t_2(22)/49 + t_2(44) + 6\{t_2(02) + t_2(20)\}/49 - \{t_2(04) + t_2(40)\}/7 - 6\{t_2(24) + t_2(42)\}/7]$$

$$i_4^{(2)} = -(\kappa/120)(\alpha/2)^9[-t_2(00)/21 + 12t_2(22)/49 + t_2(44)/3 - 6\{t_2(02) + t_2(20)\}/49 + \{t_2(04) + t_2(40)\}/7 - 2\{t_2(24) + t_2(42)\}/7]$$

$$i_{10}^{(2)} = (\kappa/20)(\alpha/2)^9[\{t_2(00) + t_2(04) + t_2(40) + t_2(44)\}/9 + 4t_2(22)/49 - 2\{t_2(02) + t_2(20) + t_2(42) + t_2(24)\}/21]$$

Let

$$u_4(2m,\ 2n) = \int_1^\infty Q_4(\lambda_1)e^{-\alpha\lambda_1/2}\lambda_1^{2m}d\lambda_1 \int_1^{\lambda_1} P_4(\lambda_2)e^{-\alpha\lambda_2/2}\lambda_2^{2n}d\lambda_2$$
$$= (1/8)[35s_4(2m,\ 2n+4) - 30s_4(2m,\ 2n+2) + 3s_4(2m,\ 2n)]$$

Then

$$i_2^{(4)} = 18c_1^4(2\pi)^2(R/2)^9(16/315)^2 \int (\lambda_1^2-1)(\lambda_2^2-1)e^{-\alpha(\lambda_1+\lambda_2)/2}Q_4\binom{\lambda_2}{\lambda_1}P_4\binom{\lambda_1}{\lambda_2}d\lambda_1 d\lambda_2$$
$$= \kappa(1/105)^2(\alpha/2)^9[u_4(00) - u_4(02) - u_4(20) + u_4(22)].$$

The other integrals for $\tau = 4$ will be somewhat similar. Since the contributions from $\tau = 2$ are small with respect to those from $\tau = 0$, the influence of $\tau = 4$ has been neglected.

$$i_6^{(1)} = -c_1^2c_2^2(2\pi)^2D_{11}(R/2)^9 \int \frac{dP_1}{d\lambda}\binom{\lambda_1}{\lambda_2}\frac{dQ_1}{d\lambda}\binom{\lambda_2}{\lambda_1}(\lambda_1^2-1)(\lambda_2^2-1)(4/3)^2$$
$$(\lambda_1^2 - \tfrac{1}{5})(\lambda_2^2 - \tfrac{1}{5})e^{-\alpha(\lambda_1+\lambda_2)/2}d\lambda_1 d\lambda_2$$
$$= (\kappa/96)(\alpha/2)^9[\{s_1(12) - s_1(10) - s_0(02) + s_0(00)\}/25 + \{s_1(34)$$
$$- s_1(32) - s_0(24) + s_0(22)\} - (\tfrac{1}{5})\{s_1(14) - s_1(12) + s_1(32) - s_1(30)$$
$$- s_0(04) + s_0(02) - s_0(22) + s_0(20)\}]$$

$$i_6^{(2)} = (3\kappa/160)(\alpha/2)^9[\{s_2(24) - s_2(22) - s_1(14) + s_1(12)\}/49 + \{s_2(46) - s_2(44)$$
$$- s_1(36) + s_1(34)\}/9 - (1/21)\{s_2(26) - s_2(24) - s_1(16) + s_1(14)$$
$$+ s_2(44) - s_2(42) - s_1(34) + s_1(32)\}]$$

$$i_{11}^{(1)} = -c_1^2c_2^2(2\pi)^2D_{11}(R/2)^9 \int (\lambda_1\mu_1 - 1)(\lambda_2\mu_2 - 1)(\lambda_1^2 - 1)(\lambda_2^2 - 1)$$
$$(\lambda_1^2 - \mu_1^2)(\lambda_2^2 - \mu_2^2)e^{-\alpha(\lambda_1+\lambda_2)/2}\frac{dP_1}{d\lambda}\binom{\lambda_1}{\lambda_2}\frac{dQ_1}{d\lambda}\binom{\lambda_2}{\lambda_1}$$
$$P_1'(\mu_1)P_1'(\mu_1)P_1'(\mu_2)P_1'(\mu_2)d\lambda_1 d\lambda_2 \cdot d\mu_1 d\mu_2$$
$$= -i_6^{(1)} \quad i_{11}^{(2)} = i_6^{(2)},\ \text{etc.}$$

For the evaluation of $i_8^{(2)}$, we use the formula

$$(\lambda^2 - 1)^2\frac{d^2Q_2}{d\lambda^2} = 2[(\lambda^2 - 1)Q_2 - \lambda Q_1 + Q_0]$$

$$i_8^{(2)} = 3c_1^4(2\pi)^2D_{22}(R/2)^9 \int (\lambda_1^2 - 1)^2(\lambda_2^2 - 1)^2\frac{d^2Q_2}{d\lambda^2}\binom{\lambda_2}{\lambda_1}(16/5)^2$$
$$(\lambda_1^2 - 1/7)(\lambda_2^2 - 1/7)e^{-\alpha(\lambda_1+\lambda_2)/2}d\lambda_1 d\lambda_2$$
$$= (\kappa/480)(\alpha/2)^9[s_2(44) + (1/7)\{s_2(04) + s_1(14)\} + s_0(24) - 8s_2(24)/7$$
$$- s_1(34) - s_0(04)/7 - (8/7)\{s_2(42) + (1/7)\{s_2(02) + s_1(12)\} + s_0(22)$$
$$- 8s_2(22)/7 - s_1(32) - s_0(02)/7\} + (1/7)\{s_2(40) + (1/7)\{s_2(00) + s_1(10)\}$$
$$+ s_0(20) - 8s_2(20)/7 - s_1(30) - s_0(00)/7\}].$$

TABLE I. $A_m(1, \alpha)$.

α	$\alpha=1.5$	2.0	2.5	3.0	3.5	4.0	4.5	5.0	6.0	7.0	8.0	9.0	10.0
$A_0(1, \alpha)$	0.14875	0.06767	0.032834	0.01660	$0.0^{2}8628$	$0.0^{2}4579$	$0.0^{2}24687$	$0.0^{2}13476$	$0.0^{3}4131$	$0.0^{3}1303$	$0.0^{4}4193$	$0.0^{4}1371$	$0.0^{5}4540$
$A_1(1, \alpha)$	.24792	.10151	.04597	.02213	.011093	$.0^{2}5724$	$.0^{2}3017$	$.0^{2}1617$	$.0^{3}4820$	$.0^{3}1489$	$.0^{4}4717$	$.0^{4}1524$	$.0^{5}4994$
$A_2(1, \alpha)$	.4793	.16917	.06961	.03135	.014967	**$.0^{2}7441$**	$.0^{2}3810$	$.0^{2}1994$	$.0^{3}5738$	$.0^{3}1728$	$.0^{4}5373$	$.0^{4}1710$	$.0^{5}5539$
$A_3(1, \alpha)$	1.1074	.32142	.11637	.04795	.02145	.010160	$.0^{2}5008$	$.0^{2}2544$	$.0^{3}6999$	$.0^{3}2043$	$.0^{4}6209$	$.0^{4}1941$	$.0^{5}6202$
$A_4(1, \alpha)$	3.1018	.7105	.21902	.08051	.03315	.01474	$.0^{2}6920$	$.0^{2}3383$	**$.0^{3}8799$**	**$.0^{3}2470$**	$.0^{4}7300$	$.0^{4}2233$	$.0^{5}7021$
$A_5(1, \alpha)$	10.488	1.844	.4709	.1508	.05598	.02300	.010158	$.0^{2}4730$	$.0^{2}11464$	$.0^{3}3067$	$.0^{4}8755$	$.0^{4}2612$	$.0^{5}8050$
$A_6(1, \alpha)$	42.10	5.599	1.1629	.3182	.10459	.03907	.016011	$.0^{2}7024$	$.0^{2}15596$	$.0^{3}3931$	$.0^{3}10760$	$.0^{4}3110$	$.0^{5}9371$
$A_7(1, \alpha)$				.7588		.07296		.01118	$.0^{2}2232$	$.0^{3}5234$	$.0^{3}1361$	$.0^{4}3790$	$.0^{4}11100$
$A_8(1, \alpha)$				2.0405		.1505		.01924	$.0^{2}3389$	$.0^{3}7285$	$.0^{3}1780$	$.0^{4}4740$	$.0^{4}1342$
$A_9(1, \alpha)$				6.138		.3432		.03598	$.0^{2}5497$	$.0^{2}10669$	$.0^{3}2422$	$.0^{4}6111$	$.0^{4}16617$
$A_{10}(1, \alpha)$				20.48		.8627		.07331	$.0^{2}9575$	$.0^{2}16544$	$.0^{3}3447$	$.0^{4}8162$	$.0^{4}2116$
$A_{11}(1, \alpha)$				75.10		2.377		.1625	.017969	$.0^{2}2730$	$.0^{3}5159$	$.0^{3}11346$	$.0^{4}2781$

TABLE II. ˙ $_1(m, \alpha)$

α	$\alpha=1.5$	2.0	2.5	3.0	3.5	4.0	4.5	5.0	6.0	7.0	8.0	9.0	10.0
$f_1(0, \alpha)$	0.05250	0.02850	0.01575	$0.0^{2}8810$	$0.0^{2}4977$	$0.0^{2}2831$	$0.0^{2}1620$	$0.0^{3}9315$	$0.0^{3}3115$	$0.0^{3}1054$	$0.0^{4}3600$	$0.0^{4}1238$	$0.0^{5}428$
$f_1(1, \alpha)$	.06535	.03425	.01846	.010141	$.0^{2}5647$	$.0^{2}3176$	$.0^{2}1800$	$.0^{2}10271$	$.0^{3}3392$	$.0^{3}1137$	$.0^{4}3854$	$.0^{4}1317$	$.0^{5}4536$
$f_1(2, \alpha)$	.08714	.04316	.02242	.011997	$.0^{2}6551$	$.0^{2}3628$	$.0^{2}2031$	$.0^{2}11473$	$.0^{3}3733$	$.0^{3}1236$	$.0^{4}4152$	$.0^{4}1409$	$.0^{5}482$
$f_1(3, \alpha)$	.1285	.05823	.02861	.014732	$.0^{2}7825$	$.0^{2}4244$	$.0^{2}2337$	$.0^{2}13028$	$.0^{3}4152$	$.0^{3}1356$	$.0^{4}4505$	$.0^{4}1516$	$.0^{5}515$
$f_1(4, \alpha)$	.2194	.0866	.03909	.019034	$.0^{2}9720$	$.0^{2}5120$	$.0^{2}2759$	$.0^{2}15105$	$.0^{3}4691$	$.0^{3}1504$	$.0^{4}4932$	$.0^{4}1643$	$.0^{5}554$
$f_1(5, \alpha)$	.455	.1474	.0587	.02635	.012722	$.0^{2}6436$	$.0^{2}3364$	$.0^{2}17986$	$.0^{3}5400$	$.0^{3}1693$	$.0^{4}5457$	$.0^{4}1795$	$.0^{5}599$
$f_1(6, \alpha)$				.03999		$.0^{2}8538$		$.0^{2}2217$	$.0^{3}6364$	$.0^{3}1936$	$.0^{4}6115$	$.0^{4}1981$	$.0^{5}653$
$f_1(7, \alpha)$				.06808		.012147		$.0^{2}2856$	$.0^{3}7727$	$.0^{3}2264$	$.0^{4}6960$	$.0^{4}2213$	$.0^{5}720$
$f_1(8, \alpha)$				.13248		.018856		$.0^{2}3894$	$.0^{3}9744$	$.0^{3}2715$	$.0^{4}8076$	$.0^{4}2507$	$.0^{5}800$
$f_1(9, \alpha)$				.2970		.03243		$.0^{2}5693$	$.0^{2}1288$	$.0^{3}3368$	$.0^{4}9595$	$.0^{4}2892$	$.0^{5}904$
$f_1(10, \alpha)$				.7642		.06244		$.0^{2}916$	$.0^{2}1805$	$.0^{3}4350$	$.0^{3}1174$	$.0^{4}3409$	$.0^{4}1036$
$f_1(11, \alpha)$				2.231		.1351		.01602	$.0^{2}2710$	$.0^{3}5906$	$.0^{3}1489$	$.0^{4}4124$	$.0^{4}1213$

The integrals $i_6^{(3)}$, $i_6^{(4)}$, and $i_8^{(4)}$ have been assumed negligible, because of the smallness of the preceding terms.

TABLE III. $\sigma_0\ (m, n, \alpha)$

α	$\alpha=3$	4	5	6	7	8	9	10
$\sigma_0(0,0,\alpha)$	0.01391	$0.0^{2}3170$	$0.0^{3}800$	$0.0^{3}2162$	$0.0^{4}611$	$0.0^{4}1787$	$0.0^{5}536$	$0.0^{5}1644$
$\sigma_0(0,2,\alpha)$	.05647	$.0^{2}9742$	$.0^{2}2043$	$.0^{3}4827$	$.0^{3}1235$	$.0^{4}3340$	$.0^{5}942$	$.0^{5}2743$
$\sigma_0(0,4,\alpha)$	.4202	.04750	$.0^{2}7474$	$.0^{2}1436$	$.0^{3}3149$	$.0^{4}7565$	$.0^{4}1942$	$.0^{5}5245$
$\sigma_0(2,0,\alpha)$	.02152	$.0^{2}445$	$.0^{2}1058$	$.0^{3}2737$	$.0^{4}7504$	$.0^{4}2143$	$.0^{6}6313$	$.0^{5}1906$
$\sigma_0(2,2,\alpha)$	.09948	.01496	$.0^{2}2884$	$.0^{3}6430$	$.0^{3}1577$	$.0^{4}4138$	$.0^{4}1138$	$.0^{5}3252$
$\sigma_0(2,4,\alpha)$	.8257	.07945	.01128	$.0^{2}2019$	$.0^{3}4203$	$.0^{4}9714$	$.0^{4}2419$	$.0^{5}6378$
$\sigma_0(4,0,\alpha)$	.04180	$.0^{2}720$	$.0^{2}1539$	$.0^{3}3717$	$.0^{4}9714$	$.0^{4}2679$	$.0^{5}768$	$.0^{5}2270$
$\sigma_0(4,2,\alpha)$	.2438	.02824	$.0^{2}4674$	$.0^{3}9446$	$.0^{3}2168$	$.0^{4}5417$	$.0^{4}1438$	$.0^{5}3995$
$\sigma_0(4,4,\alpha)$	2.4886	.1748	.02051	$.0^{2}3237$	$.0^{3}6183$	$.0^{3}13424$	$.0^{4}3192$	$.0^{5}8122$

TABLE IV. $s_0(m,n,\alpha)$

α	$\alpha=3$	4	5	6	7	8	9	10
$S_0(0,0,\alpha)$	$0.0^{2}753$	$0.0^{2}1798$	$0.0^{3}470$	$0.0^{3}1302$	$0.0^{4}375$	$0.0^{4}1117$	$0.0^{5}340$	$0.0^{5}1055$
$S_0(0,2,\alpha)$	.01261	$.0^{2}2678$	$.0^{3}650$	$.0^{3}1715$	$.0^{4}476$	$.0^{4}1378$	$.0^{5}410$	$.0^{5}1251$
$S_0(0,4,\alpha)$	.0268	$.0^{2}466$	$.0^{2}1000$	$.0^{3}243$	$.0^{4}640$	$.0^{4}1780$	$.0^{5}514$	$.0^{5}1528$
$S_0(2,0,\alpha)$	.02508	$.0^{2}474$	$.0^{2}1058$	$.0^{3}2620$	$.0^{4}694$	$.0^{4}1933$	$.0^{5}5580$	$.0^{5}1659$
$S_0(2,2,\alpha)$	.05069	$.0^{2}800$	$.0^{2}1601$	$.0^{3}370$	$.0^{4}928$	$.0^{4}2485$	$.0^{5}697$	$.0^{5}2023$
$S_0(2,4,\alpha)$	.1460	.01700	$.0^{2}283$	$.0^{3}580$	$.0^{3}1345$	$.0^{4}3405$	$.0^{5}914$	$.0^{5}2569$
$S_0(4,0,\alpha)$	.1421	.01849	$.0^{2}3221$	$.0^{3}669$	$.0^{3}1555$	$.0^{4}3917$	$.0^{4}1045$	$.0^{5}2916$
$S_0(4,2,\alpha)$	.3485	.03599	$.0^{2}5417$	$.0^{2}1022$	$.0^{3}2214$	$.0^{4}5301$	$.0^{4}1360$	$.0^{5}3681$
$S_0(4,4,\alpha)$	1.345	.0949	.01124	$.0^{2}1812$	$.0^{3}3520$	$.0^{4}7803$	$.0^{4}1891$	$.0^{5}490$

TABLE V. $\sigma_1(m,n,\alpha)$

α	$\alpha=3$	4	5	6	7	8	9	10
$\sigma_1(1,0,\alpha)$	$0.0^{2}6761$	$0.0^{2}1588$	$0.0^{3}41080$	$.0^{3}11307$	$0.0^{4}3249$	$0.0^{5}9636$	$0.0^{5}2927$	$0.0^{6}907$
$\sigma_1(1,2,\alpha)$	.02649	$.0^{2}4730$	$.0^{2}10197$	$.0^{3}2464$	$.0^{4}6422$	$.0^{4}1765$	$.0^{5}5049$	$.0^{5}1488$
$\sigma_1(1,4,\alpha)$	.1927	.02253	$.0^{2}3644$	$.0^{3}7171$	$.0^{3}1604$	$.0^{4}3921$	$.0^{4}10227$	$.0^{5}2799$
$\sigma_1(1,6,\alpha)$	2.7214	.18784	.020763	$.0^{2}3072$	$.0^{3}5523$	$.0^{3}11383$	$.0^{4}2594$	$.0^{5}6367$
$\sigma_1(3,0,\alpha)$	$.0^{2}9821$	$.0^{2}2122$	$.0^{3}5211$	$.0^{3}1384$	$.0^{4}3874$	$.0^{4}11264$	$.0^{5}3369$	$.0^{5}1030$
$\sigma_1(3,2,\alpha)$	.04322	$.0^{2}6839$	$.0^{2}13697$	$.0^{3}3150$	$.0^{4}7926$	$.0^{4}2121$	$.0^{5}5944$	$.0^{5}1722$
$\sigma_1(3,4,\alpha)$	.3470	.03513	$.0^{2}5194$	$.0^{3}9602$	$.0^{3}2055$	$.0^{4}4860$	$.0^{4}12354$	$.0^{5}3311$
$\sigma_1(3,6,\alpha)$	5.177	.3079	.03096	$.0^{2}4280$	$.0^{3}7327$	$.0^{3}1454$	$.0^{4}3217$	$.0^{5}7703$

TABLE VI. $s_1\ (m, n, \alpha)$

α	$\alpha=3$	4	5	6	7	8	9	10
$S_1(1,0,\alpha)$	$0.0^{2}2959$	$0.0^{3}730$	$0.0^{3}1953$	$0.0^{4}5525$	$0.0^{4}1623$	$0.0^{5}4907$	$0.0^{5}1518$	$0.0^{6}477$
$S_1(1,2,\alpha)$	$.0^{2}482$	$.0^{2}1064$	$.0^{3}2653$	$.0^{4}715$	$.0^{4}2030$	$.0^{5}599$	$.0^{5}1808$	$.0^{6}5607$
$S_1(1,4,\alpha)$	$.0^{2}998$	$.0^{2}1804$	$.0^{3}399$	$.0^{4}994$	$.0^{4}2678$	$.0^{5}760$	$.0^{5}2230$	$.0^{6}676$
$S_1(1,6,\alpha)$	.0296	$.0^{2}390$	$.0^{3}705$	$.0^{3}1544$	$.0^{4}383$	$.0^{4}103$	$.0^{5}2885$	$.0^{6}847$
$S_1(3,0,\alpha)$	$.0^{2}929$	$.0^{2}1818$	$.0^{3}4182$	$.0^{3}10612$	$.0^{4}2877$	$.0^{5}8169$	$.0^{5}2401$	$.0^{6}7253$
$S_1(3,2,\alpha)$	.01837	$.0^{2}300$	$.0^{3}6216$	$.0^{3}1468$	$.0^{4}3786$	$.0^{4}1037$	$.0^{5}2960$	$.0^{6}877$
$S_1(3,4,\alpha)$	.0516	$.0^{2}625$	$.0^{2}1070$	$.0^{3}2259$	$.0^{4}538$	$.0^{4}1395$	$.0^{5}3821$	$.0^{5}1096$
$S_1(3,6,\alpha)$	.232	.0176	$.0^{2}230$	$.0^{3}407$	$.0^{4}857$	$.0^{4}204$	$.0^{5}526$	$.0^{5}1448$

RESULTS

The results have been tabulated in Tables I–XV. The values are based partly on integral logarithm tables given by Jahnke–Emde, and the accuracy is limited thereby. The tables are, therefore, subject to revision on this account. Except for this, they are accurate up to a possible change of the last figure. In this connection, it is urged that the tabular method is the economical one, in that the calculations may be checked easily.

TABLE VII. $\sigma_2(m,n,\alpha)$

α	$\alpha=3$	4	5	6	7	8	9	10
$\sigma_2(0,0,\alpha)$	$0.0^{2}3185$	$0.0^{3}797$	$0.0^{3}2158$	$0.0^{4}6154$	$0.0^{4}1818$	$0.0^{5}552$	$0.0^{5}1709$	$0.0^{6}540$
$\sigma_2(0,2,\alpha)$	.011511	$.0^{2}2225$	$.0^{3}5079$	$.0^{3}12825$	$.0^{4}3459$	$.0^{5}979$	$.0^{5}2865$	$.0^{5}0861$
$\sigma_2(0,4,\alpha)$	.0792	.01004	$.0^{2}1729$	$.0^{3}3574$	$.0^{4}8318$	$.0^{4}2099$	$.0^{5}5628$	$.0^{5}1576$
$\sigma_2(0,6,\alpha)$	1.092	.0814	$.0^{2}955$	$.0^{2}1484$	$.0^{3}2777$	$.0^{4}5917$	$.0^{4}1388$	$.0^{5}3492$
$\sigma_2(2,0,\alpha)$	$.0^{2}3976$	$.0^{3}958$	$.0^{3}2528$	$.0^{4}708$	$.0^{4}2060$	$.0^{5}618$	$.0^{5}1897$	$.0^{6}593$
$\sigma_2(2,2,\alpha)$	.01511	$.0^{2}2775$	$.0^{3}6130$	$.0^{3}1510$	$.0^{4}4001$	$.0^{4}1113$	$.0^{5}3224$	$.0^{6}960$
$\sigma_2(2,4,\alpha)$	.10773	.01295	$.0^{2}2147$	$.0^{3}4311$	$.0^{4}981$	$.0^{4}2433$	$.0^{5}6432$	$.0^{5}1780$
$\sigma_2(2,6,\alpha)$	1.509	.1069	.01209	$.0^{2}1823$	$.0^{3}3335$	$.0^{4}6970$	$.0^{4}1609$	$.0^{5}3991$
$\sigma_2(4,0,\alpha)$	$.0^{2}545$	$.0^{2}1224$	$.0^{3}310$	$.0^{4}8415$	$.0^{4}2401$	$.0^{5}7066$	$.0^{5}2142$	$.0^{6}663$
$\sigma_2(4,2,\alpha)$	.02296	$.0^{2}3799$	$.0^{3}789$	$.0^{3}1862$	$.0^{4}4789$	$.0^{4}1305$	$.0^{5}3712$	$.0^{5}1090$
$\sigma_2(4,4,\alpha)$	.1787	.01892	$.0^{2}2904$	$.0^{3}5533$	$.0^{3}1214$	$.0^{4}2926$	$.0^{5}7566$	$.0^{5}2053$
$\sigma_2(4,6,\alpha)$	2.63	.1628	.01729	$.0^{2}2418$	$.0^{3}4247$	$.0^{4}8588$	$.0^{4}1937$	$.0^{5}4696$

TABLE VIII. $s_2(m,n,\alpha)$

α	$\alpha=3$	4	5	6	7	8	9	10
$S_2(0,0,\alpha)$	$0.0^{3}677$	$0.0^{3}195$	$0.0^{4}582$	$0.0^{4}1778$	$0.0^{5}558$	$0.0^{5}178$	$0.0^{6}577$	$0.0^{6}187$
$S_2(0,2,\alpha)$	$.0^{3}93$	$.0^{3}255$	$.0^{4}728$	$.0^{4}216$	$.0^{5}664$	$.0^{5}208$	$.0^{6}662$	$.0^{6}214$
$S_2(0,4,\alpha)$	$.0^{2}135$	$.0^{3}37$	$.0^{4}98$	$.0^{4}274$	$.0^{5}81$	$.0^{5}251$	$.0^{6}778$	$.0^{6}249$
$S_2(0,6,\alpha)$	$.0^{2}12$	$.0^{2}07$	$.0^{3}150$	$.0^{4}373$	$.0^{4}104$	$.0^{5}313$	$.0^{6}94$	$.0^{6}298$
$S_2(2,0,\alpha)$	$.0^{2}139$	$.0^{3}360$	$.0^{4}983$	$.0^{4}282$	$.0^{5}845$	$.0^{5}259$	$.0^{6}811$	$.0^{6}259$
$S_2(2,2,\alpha)$	$.0^{2}22$	$.0^{3}51$	$.0^{3}131$	$.0^{4}360$	$.0^{4}1037$	$.0^{5}313$	$.0^{6}957$	$.0^{6}300$
$S_2(2,4,\alpha)$	$.0^{2}43$	$.0^{3}88$	$.0^{3}195$	$.0^{4}491$	$.0^{4}1345$	$.0^{5}391$	$.0^{5}1162$	$.0^{6}359$
$S_2(2,6,\alpha)$	.011	$.0^{2}21$	$.0^{3}35$	$.0^{4}75$	$.0^{4}187$	$.0^{5}52$	$.0^{5}147$	$.0^{6}449$
$S_2(4,0,\alpha)$	$.0^{2}41$	$.0^{3}893$	$.0^{3}201$	$.0^{4}518$	$.0^{4}143$	$.0^{5}415$	$.0^{5}1247$	$.0^{6}381$
$S_2(4,2,\alpha)$	$.0^{2}79$	$.0^{2}1494$	$.0^{3}295$	$.0^{4}705$	$.0^{4}186$	$.0^{5}517$	$.0^{5}1517$	$.0^{6}455$
$S_2(4,4,\alpha)$	.021	$.0^{2}331$	$.0^{3}51$	$.0^{3}1061$	$.0^{4}260$	$.0^{5}683$	$.0^{5}1932$	$.0^{6}568$
$S_2(4,6,\alpha)$	.08	.0124	$.0^{3}81$	$.0^{3}188$	$.0^{4}41$	$.0^{5}98$	$.0^{5}261$	$.0^{6}745$

TABLE IX. $S_{mm}'(\alpha/2)$, *etc.*

α	$\alpha=3$	4	5	6	7	8	9	10
$(S_{00})^{1/2}$	0.4825	0.2256	$0.0^{2}5086$	−0.1597	−0.2649	−0.3187	−0.3326	−0.3190
S_{00}	.2328	.05088	$.0^{4}2587$	.02556	.07020	.10156	.11062	.10174
$(S_{11})^{1/2}$	.8089	.6947	.5778	.4679	.3702	.2871	.2185	.16405
S_{11}	.6542	.4826	.3339	.2189	.13695	.08241	.04774	.02692
S_{10}	.3903	.1567	$.0^{2}2939$	−.0747	−.09807	−.09147	−.07268	−.05233

In order not to make the labor prohibitive in other cases, some more straightforward method should be employed to obtain the entries for $s_2(m, n, \alpha)$ and similar quantities. As it is, the accuracy for small values of α is quite small. This is not serious, however, for the approximation method itself can be expected to give good results only for large values of the internuclear distance.

Table X. *List of Integrals*

	$\nu = 0$	$\nu = 1$	$\nu = 2$	$\nu = 3$	$\nu = 4$
$\int_{-1}^{1} (\lambda + \mu)^3(\lambda - \mu)^\nu d\mu$	$2\lambda(\lambda^2 + 1)$	$2\left(\lambda^4 - \frac{1}{5}\right)$	$2\lambda\left(\lambda^4 - \frac{2}{3}\lambda^2 + \frac{1}{5}\right)$	$2\left(\lambda^6 - \lambda^4 + \frac{3}{5}\lambda^2 - \frac{1}{7}\right)$	$2\lambda\left(\lambda^6 - \lambda^4 + \frac{3}{5}\lambda^2 - \frac{1}{7}\right)$
$\int (1-\mu^2)^2(\lambda+\mu)(\lambda-\mu)^\nu d\mu$	$\frac{16}{15}\lambda$	$\frac{16}{15}\left(\lambda^2 - \frac{1}{7}\right)$	$\frac{16}{15}\lambda\left(\lambda^2 - \frac{1}{7}\right)$		
$\int (\lambda\mu + 1)^2(\lambda + \mu) \cdot (\lambda - \mu)^\nu d\mu$	$\frac{2}{3}\lambda(\lambda^2 + 5)$	$\frac{2}{3}\lambda^4 + \frac{8}{5}\lambda^2 - \frac{2}{3}$	$\frac{2}{3}\lambda^5 + \frac{4}{15}\lambda^3 + \frac{2}{15}\lambda$	$\frac{2}{3}\lambda^6 - \frac{2}{3}\lambda^4 + \frac{46}{35}\lambda^2 - \frac{2}{5}$	$\frac{2}{3}\lambda^7 - \frac{6}{5}\lambda^5 + \frac{218}{105}\lambda^3 - \frac{22}{35}\lambda$
$\int (\lambda\mu + 1)^2(\lambda + \mu) (1 - \mu^2)(\lambda - \mu)^\nu d\mu$	$\frac{4}{15}\lambda^3 + \frac{28}{15}\lambda$	$\frac{4}{15}\lambda^4 + \frac{128}{105}\lambda^2 - \frac{4}{15}$	$\frac{4}{15}\lambda^5 + \frac{24}{35}\lambda^3 - \frac{4}{105}\lambda$		
$\int (1 - \mu^2)(\lambda + \mu)^3 \cdot (\lambda - \mu)^\nu d\mu$	$\frac{4}{3}\lambda^3 + \frac{12}{15}\lambda$	$\frac{4}{3}\lambda^4 - \frac{4}{35}$	$\frac{4}{3}\lambda^5 - \frac{8}{15}\lambda^3 + \frac{4}{35}\lambda$		
$\int (1-\mu^2)(\lambda+\mu) \cdot (\lambda-\mu)^\nu d\mu$	$\frac{4}{3}\lambda$	$\frac{4}{3}\lambda^2 - \frac{4}{15}$	$\frac{4}{3}\lambda^3 - \frac{4}{15}\lambda$	$\frac{4}{3}\lambda^4 - \frac{4}{35}$	$\frac{4}{3}\lambda^5 + \frac{8}{15}\lambda^3 - \frac{12}{35}\lambda$
$\int (1 - \mu^2)(\lambda^2\mu^2 - 1) \cdot (\lambda + \mu)(\lambda - \mu)^\nu d\mu$	$\frac{4}{15}\lambda^3 - \frac{4}{3}\lambda$	$\frac{4}{15}\lambda^4 - \frac{152}{105}\lambda^2 + \frac{4}{15}$	$\frac{4}{15}\lambda^5 - \frac{152}{105}\lambda^3 + \frac{4}{15}\lambda$		
$\int (\lambda\mu - 1)(\lambda^2 - \mu^2) \cdot (1 - \mu^2) d\mu$	$-\frac{4}{3}\left(\lambda^2 - \frac{1}{5}\right)$				
$\int (\lambda + \mu)^3(\lambda\mu - 1)^2 (\lambda - \mu)^\nu d\mu$	$\frac{2}{3}\lambda^5 - \frac{4}{5}\lambda^3 + \frac{6}{5}\lambda$	$\frac{2}{3}\lambda^6 - \frac{2}{3}\lambda^4 + \frac{46}{35}\lambda^2 - \frac{2}{5}$	$\frac{2}{3}\lambda^7 - \frac{2}{15}\lambda^5 + \frac{58}{105}\lambda^3 - \frac{6}{35}\lambda$		

List of Integrals (cont'd.)

	$\nu = 1$	$\nu = 2$	$\nu = 3$	$\nu = 4$
$\int_{-1}^{1} \frac{d\mu}{(\lambda-\mu)^{\nu}}$	$2Q_0$	$\frac{2}{\lambda^2-1} = -2Q_0'$	$\frac{2\lambda}{(\lambda^2-1)^2} = Q_0''$	$\frac{2}{3}\frac{3\lambda^2+1}{(\lambda^2-1)^3} = -\frac{1}{3}Q_0'''$
$\int \frac{\lambda+\mu}{(\lambda-\mu)^{\nu}} d\mu$	$4\lambda Q_0 - 2 = 4Q_1 + 2$	$\frac{4\lambda}{\lambda^2-1} - 2Q_0$	$\frac{2(\lambda^2+1)}{(\lambda^2-1)^2} = 2(\lambda Q_0'' + Q_0')$	$\frac{1}{3}\{-3Q_0'' - 2\lambda Q_0'''\}$
		$= -2Q_0 - 4\lambda Q_0'$	$= 2(Q_1'' - Q_0')$	$= \frac{6\lambda^3+10\lambda}{3(\lambda^2-1)^3}$
$\int \frac{(\lambda+\mu)^2}{(\lambda-\mu)^{\nu}} d\mu$	$8\lambda Q_1 + 2\lambda$	$\frac{8}{\lambda^2-1} + 10 - 8\lambda Q_0$	$\frac{8\lambda}{(\lambda^2-1)^2} + 2Q_0$	$\frac{32}{3}\cdot\frac{1}{(\lambda^2-1)^3} + \frac{32}{3(\lambda^2-1)^2} + \frac{2}{\lambda^2-1}$
$\int \frac{(\lambda+\mu)^3}{(\lambda-\mu)^{\nu}} d\mu$	$16\lambda^2 Q_1 + 2\lambda^2 - \frac{2}{3}$	$10\lambda - 24\lambda^2 Q_0 + \frac{16\lambda^3}{\lambda^2-1}$	$12\lambda Q_0 - 10 + \frac{8(\lambda^2+1)}{(\lambda^2-1)^2}$	$\frac{64\lambda}{3(\lambda^2-1)^3} + \frac{40\lambda}{3(\lambda^2-1)^2}$
		$= -24\lambda Q_1 + 2\lambda + \frac{16\lambda}{\lambda^2-1}$		$+ \frac{4\lambda}{\lambda^2-1} - 2Q_0$
$\int \frac{1-\mu^2}{(\lambda-\mu)^{\nu}} d\mu$	$2Q_0 - 2\lambda Q_1 = -2Q_1'(\lambda^2-1)$	$4Q_1$	$\frac{2\lambda}{\lambda^2-1} - 2Q_0 = \frac{2Q_0 - 2\lambda Q_1}{\lambda^2-1}$	$\frac{4}{3(\lambda^2-1)^2} = \frac{2}{3}Q_1''$
			$= -2Q_1'$	
$\int \frac{(1-\mu^2)^2}{(\lambda-\mu)^{\nu}} d\mu$	$(2\lambda^3 - 4\lambda)Q_1 + 2Q_0 - \frac{2}{3}\lambda$	$8\left\{(1-\lambda^2)Q_1 + \frac{1}{3}\right\}$	$8Q_2$	$-8Q_1 + \frac{8}{3(\lambda^2-1)} = -\frac{8}{3}Q_2'$
	$= (\lambda^2-1)^2 Q_0 - 4\lambda(\lambda^2-1)$	$= -\frac{8}{3}Q_2'(\lambda^2-1)$		
	$+ 2\lambda\left(\lambda^2 - \frac{1}{3}\right)$			
$\int \frac{(\lambda\mu+1)^2}{(\lambda-\mu)^{\nu}} d\mu$	$2\lambda^3 Q_1 + 4\lambda Q_1 + 2Q_0$	$-4\lambda^2 Q_1 - 4Q_1 - 6 + \frac{8\lambda^2}{\lambda^2-1}$	$2\lambda Q_1 + \frac{8\lambda}{(\lambda^2-1)^2}$	$\frac{32}{3(\lambda^2-1)^3} + \frac{32}{3(\lambda^2-1)^2} + \frac{2}{3(\lambda^2-1)}$
$\int \frac{(\lambda^2\mu^2-1)}{(\lambda-\mu)^{\nu}} d\mu$	$2\lambda^3 Q_1 - 2Q_0$	$-4\lambda^2 Q_1 + 2$	$2\lambda Q_1$	$\frac{2}{3}\frac{\lambda^2+1}{(\lambda^2-1)^2} = \frac{2}{3}\cdot\frac{1}{\lambda^2-1}$
				$+ \frac{4}{3(\lambda^2-1)^2}$

List of Integrals (cont'd.)

	$\nu = 1$	$\nu = 2$	$\nu = 3$	$\nu = 4$
$\int \frac{\lambda\mu+1}{(\lambda-\mu)^\nu}d\mu$	$2\lambda Q_1 + 2Q_0$	$-2Q_1+\frac{4}{\lambda^2-1}$	$\frac{4\lambda}{(\lambda^2-1)^2}$	$\frac{14}{3(\lambda^2-1)^2}+\frac{16}{3(\lambda^2-1)^3}$
$\int \frac{(\lambda\mu+1)^2(1-\mu^2)}{(\lambda-\mu)^\nu}d\mu$	$(1-\lambda^2)(2\lambda^2Q_1+4\lambda Q_1+2Q_0)+\frac{2}{3}\lambda^3$ $+\frac{10}{3}\lambda=(-2\lambda^5-2\lambda^3+2\lambda)Q_1$ $+2Q_0+\frac{2}{3}\lambda^3+\frac{4}{3}\lambda$	$\frac{8}{3}(\lambda^2+1)(3\lambda^2Q_1-1)-\frac{4}{3}$ $=(8\lambda^4+8\lambda^2)Q_1-\frac{8}{3}\lambda^2-4$	$-12\lambda^3Q_1-10\lambda Q_1+4\lambda-2Q_0$ $+\frac{8\lambda}{\lambda^2-1}$	$8\lambda^2Q_1+4Q_1-\frac{8}{3}-\frac{8}{3(\lambda^2-1)}$ $+\frac{16}{3(\lambda^2-1)^2}$
$\int \frac{(1-\mu^2)(\lambda+\mu)^2}{(\lambda-\mu)^\nu}d\mu$	$-8\lambda^3Q_1+8\lambda Q_1+4\lambda$	$(24\lambda^2-8)Q_1-\frac{20}{3}$	$-26\lambda Q_1+2Q_0+\frac{8\lambda}{\lambda^2-1}$	$12Q_1+\frac{16}{3(\lambda^2-1)^2}-\frac{8}{3(\lambda^2-1)}$
$\int \frac{(\lambda^2\mu^2-1)(1-\mu^2)}{(\lambda-\mu)^\nu}d\mu$	$(-2\lambda^5+2\lambda^3+2\lambda)Q_1-2Q_0+\frac{2}{3}\lambda^3$	$(8\lambda^4-4\lambda^2-4)Q_1-\frac{8}{3}\lambda^2$	$-12\lambda^3Q_1+2\lambda Q_1+4\lambda+2Q_0$	$8\lambda^2Q_1-\frac{8}{3}-\frac{4}{3}\cdot\frac{1}{\lambda^2-1}$
$\int \frac{(\lambda\mu+1)(1-\mu^2)}{(\lambda-\mu)^\nu}d\mu$	$-2\lambda^3Q_1+2Q_0+\frac{2}{3}\lambda$	$6\lambda^2Q_1+2Q_1-2$	$-6\lambda Q_1-2Q_0+\frac{4\lambda}{\lambda^2-1}$	$2Q_1-\frac{2}{3(\lambda^2-1)}+\frac{8}{3(\lambda^2-1)^2}$
$\int \frac{(\lambda\mu+1)(\lambda+\mu)}{(\lambda-\mu)^\nu}d\mu$	$4\lambda^2Q_1+4Q_1+2$	$-6\lambda Q_1-2Q_0+\frac{8\lambda}{\lambda^2-1}$	$2Q_1+\frac{4}{\lambda^2-1}+\frac{8}{(\lambda^2-1)^2}$	$\frac{32\lambda}{3(\lambda^2-1)^3}+\frac{16\lambda}{3(\lambda^2-1)^2}$
$\int \frac{(\lambda^2\mu^2-1)(\lambda+\mu)(1-\mu^2)}{(\lambda-\mu)^\nu}d\mu$	$(-2\lambda^6+2\lambda^4+2\lambda^2-2)\cdot 2Q_1$ $+\frac{4}{3}\lambda^4-\frac{4}{15}\lambda^2-\frac{8}{3}$	$18\lambda^5Q_1-10\lambda^3Q_1-10\lambda Q_1$ $-6\lambda^3+2Q_0$	$-32\lambda^4Q_1+8\lambda^2Q_1+8Q_1$ $+\frac{32}{3}\lambda^2+4$	$28\lambda^3Q_1-2\lambda Q_1-\frac{28}{3}\lambda-2Q_0$ $-\frac{8}{3}\cdot\frac{\lambda}{\lambda^2-1}$
$\int \frac{(1-\mu^2)^2(\lambda+\mu)}{(\lambda-\mu)^\nu}d\mu$	$4(\lambda^2-1)^2Q_1+\frac{8}{5}-\frac{4}{3}(\lambda^2-1)$	$-18\lambda^3Q_1+20\lambda Q_1+6\lambda-2Q_0$	$32\lambda^2Q_1-16Q_1-\frac{32}{3}$	$-28\lambda Q_1+4Q_0+\frac{16}{3}\cdot\frac{\lambda}{\lambda^2-1}$

List of Integrals (cont'd.)

	$\nu = 1$	$\nu = 2$	$\nu = 3$	$\nu = 4$
$\int \frac{(\lambda\mu + 1)^2(1 - \mu^2)(\lambda + \mu)}{(\lambda - \mu)^\nu} d\mu$	$(-4\lambda^6 - 4\lambda^4 + 4\lambda^2 + 4)Q_1 + \frac{4}{3}\lambda^4 + \frac{12}{5}\lambda^2 - \frac{8}{3}$	$(18\lambda^5 + 18\lambda^3 - 2\lambda)Q_1 - 6\lambda^3 - \frac{28}{3}\lambda - 2Q_0$	$(-32\lambda^4 - 28\lambda^2 - 4)Q_1 + \frac{32}{3}\lambda^2 + \frac{16\lambda^2}{\lambda^2 - 1}$	$28\lambda^3 Q_1 + 18\lambda Q_1 - \frac{28}{3}\lambda + 2Q_0 - \frac{40}{3}\cdot\frac{\lambda}{\lambda^2 - 1} + \frac{32}{3}\cdot\frac{\lambda}{(\lambda^2 - 1)^2}$
$\int \frac{(\lambda\mu + 1)^2(\lambda + \mu)}{(\lambda - \mu)^\nu} d\mu$	$(4\lambda^4 + 8\lambda^2 + 4)Q_1 + 2 - \frac{2}{3}\lambda^2$	$-10\lambda^3 Q_1 - 12\lambda Q_1 + 4\lambda - 2Q_0 + \frac{16\lambda}{\lambda^2 - 1}$	$-8\lambda^2 - 6 + \frac{8(\lambda^2 + 1)}{(\lambda^2 - 1)^2} + 8\lambda^3 Q_0 + 4\lambda Q_0$	
$\int \frac{(\lambda + \mu)^3(1 - \mu^2)}{(\lambda - \mu)^\nu} d\mu$	$-16\lambda^4 Q_1 + 16\lambda^2 Q_1 + \frac{20}{3}\lambda^2 - \frac{4}{15}$	$56\lambda^3 Q_1 - 24\lambda Q_1 - \frac{52}{3}\lambda$	$-76\lambda^2 Q_1 + 12Q_1 + \frac{32}{3} + \frac{16\lambda^2}{\lambda^2 - 1}$	$50\lambda Q_1 - 2Q_0 - \frac{40}{3}\frac{\lambda}{\lambda^2 - 1} + \frac{32}{3}\cdot\frac{\lambda}{(\lambda^2 - 1)^2}$
$\int \frac{(1 - \mu^2)(\lambda + \mu)}{(\lambda - \mu)^\nu} d\mu$	$-4\lambda^2 Q_1 + 4Q_1 + \frac{8}{3}$	$10\lambda Q_1 - 2Q_0$	$-8Q_1 + \frac{4}{\lambda^2 - 1}$	
$\int \frac{(1 - \mu^2)(\lambda + \mu)^2}{(\lambda - \mu)^\nu} d\mu$	$-8\lambda^3 Q_1 + 8\lambda Q_1 + 4\lambda$			
$\int \frac{(\lambda + \mu)^3(\lambda\mu - 1)^2}{(\lambda - \mu)^\nu} d\mu$	$(1 - \lambda^2)^2 \cdot 16\lambda^2 Q_1 - \frac{14}{3}\lambda^4 + \frac{104}{15}\lambda^2 - \frac{2}{3}$	$(-56\lambda^5 + 80\lambda^3 - 24\lambda)Q_1 + \frac{58}{3}\lambda^3 - \frac{46}{3}\lambda$	$(76\lambda^4 - 72\lambda^2 + 12)Q_1 - \frac{74}{3}\lambda^2 + 10$	$(-50\lambda^3 + 28\lambda)Q_1 - 2Q_0 + \frac{16\lambda}{3(\lambda^2 - 1)} + \frac{52\lambda}{3}.$

TABLE XI. *List of Integrals*

	$R > a^2$	$R < a$
$\int_{\lvert R-a \rvert}^{R+a} db$	$2a$	$2R$
$\int b^2 db$	$2a\left(R^2 + \frac{a^2}{3}\right)$	$2R\left(a^2+\frac{R^2}{3}\right)$
$\int b^4 db$	$2a\left(R^4 + 2a^2R^2 + \frac{1}{5}a^4\right)$	$2R\left(a^4 + 2R^2a^2 + \frac{1}{5}R^4\right)$
$\int \frac{db}{b^2}$	$\frac{2a}{R^2 - a^2}$	$\frac{2R}{a^2 - R^2}$
$\int \frac{db}{b^4}$	$2a\frac{(R^2 + a^2/3)}{(R^2 - a^2)^3}$	$2R\frac{(a^2 + R^2/3)}{(a^2 - R^2)^3}$
$\int \sin^2\theta_b db$ $= \int a^2 \sin^2 \theta_a \cdot db/b^2$	$\frac{4a^3}{3R^2}$	$\frac{4}{3}R$
$\int \sin^2 \theta_b \cdot b^2 db$ $= \int a^2 \sin^2 \theta_a db$	$\frac{4a^3}{3R^2}\left(R^2 - \frac{a^2}{5}\right)$	$\frac{4}{3} R \left(a^2 - \frac{R^2}{5}\right)$
$\int \sin^2 \theta_b \cdot \frac{db}{b^2}$ $= \int a^2 \sin^2 \theta_a \cdot \frac{db}{b^4}$	$\frac{4}{3} \frac{a^3}{R^2} \cdot \frac{1}{R^2 - a^2}$	$\frac{4}{3}R \cdot \frac{1}{a^2 - R^2}$
$\int \sin^4 \theta_b db$ $= \int a^2 \sin^2 \theta_a \sin^2 \theta_b \cdot \frac{db}{b^2}$	$\frac{16}{15} \frac{a^5}{R^4}$	$\frac{16}{15}R$
$\int \frac{a^2 \cos^2 \theta_a}{b^2} db$	$\frac{2a}{R^2 - a^2} \cdot \frac{a^2}{3R^2} \cdot (2a^2 + R^2)$	$\frac{2R}{a^2 - R^2} \cdot \frac{1}{3}(a^2+2R^2) = \frac{2}{3}R + \frac{2R^3}{a^2 - R^2}$
$\int P_2(\cos \theta_a) \cdot \frac{db}{b^2}$	$\frac{2a}{R^2 - a^2} \cdot \frac{a^2}{R^2}$	$\frac{2R}{a^2 - R^2} \cdot \frac{R^2}{a^2}$
$\int \frac{a^2 \cos^2 \theta_a \sin^2 \theta_b}{b^2} db$	$\frac{4a^5}{3R^4}\left(\frac{R^2 + 4a^2}{5(R^2 - a^2)}\right)$	$\frac{4}{3}R \cdot \frac{a^2 + 4R^2}{5(a^2 - R^2)} = \frac{4}{15}R + \frac{4}{3} \frac{R^3}{a^2 - R^2}$
$\int \cos^2 \theta_b db$	$2a - \frac{4a^3}{3R^2}$	$2R - \frac{4}{3}R = \frac{2}{3}R$
$\int \cos^2 \theta_a db$	$\frac{2a}{3R^2}\left(\frac{2}{5}a^2 + R^2\right)$	$\frac{2}{3} \cdot \frac{R}{a^2}\left(\frac{2}{5}R^2 + a^2\right)$
$\int P_2(\cos \theta_a) db$	$\frac{2}{5} \frac{a^3}{R^2}$	$\frac{2}{5} \frac{R^3}{a^2}$
$\int a^2 \sin \theta_a \sin \theta_b \cdot \cos \theta_a \cos \theta_b \cdot \frac{db}{b^2}$	$-\frac{16}{15} \frac{a^5}{R^4}$	$+\frac{4}{15}R$
$\int \frac{ab \cos \theta_a \cos \theta_b}{b^2} db$	$-\frac{4a^3}{3R^2}$	$+\frac{2}{3}R$
$\int \frac{a^2 \cos^2 \theta_a \cos^2 \theta_b}{b^2} db$	$\frac{2}{3} \frac{a^3}{R^2 - a^2} + \frac{16}{15} \frac{a^5}{R^4}$	$\frac{2}{3} \frac{Ra^2}{a^2 - R^2} - \frac{4}{15}R$
$\int \frac{a^2 \sin^2 \theta_a \cos^2 \theta_b}{b^2} db$	$\frac{4}{3} \frac{a^3}{R^2} - \frac{16}{15} \frac{a^5}{R^4}$	$\frac{4}{15}R$
$\int \frac{a^2 \cos^2 \theta_b}{b^2} db$	$\frac{2}{3} \frac{a^3}{R^2 - a^2} + \frac{4}{3} \frac{a^3}{R^2}$	$\frac{2}{3} \frac{Ra^2}{a^2 - R^2}$

TABLE XII. *Numerical Results*

			3	4	5	6	7	8	9	10
I	(a)	$(\kappa^5/2\pi)\int a^2 \sin^2\theta_a e^{-\kappa a}(\Gamma_5/\kappa b)dv$	154.0	137.0	121.4	108.0	96.8	87.1	79.0	72.1
	(b)	$(\kappa^5/2\pi)\int a^2 \sin^2\theta_a e^{-\kappa a}[\Gamma_5(\kappa b)/\kappa b - \Gamma_4(\kappa b)]dv$	26.8	17.7	10.9	6.5	3.7	2.0	1.1	0.6
	(c)	$(\kappa^5/2\pi)\int a^2 \sin^2\theta_a e^{-\kappa a}g_{5,1}dv$	127.2	119.3	110.5	101.5	93.1	85.1	77.9	71.5
II	(a)	$(\kappa^5/2\pi)\int a^2 \cos^2\theta_a e^{-\kappa a}(\Gamma_5/\kappa b)dv$	103.1	94.6	83.6	72.6	62.9	54.6	48.0	42.6
	(b)	$(\kappa^5/2\pi)\int a^2 \cos^2\theta_a e^{-\kappa a}[\Gamma_5(\kappa b)/\kappa b - \Gamma_4(\kappa b)]dv$	36.7	31.0	23.3	16.1	10.4	6.4	3.8	2.1
	(c)	$(\kappa^5/2\pi)\int a^2 \cos^2\theta_a e^{-\kappa a}g_{5,1}dv$	66.4	63.6	60.3	56.5	52.5	48.8	44.2	40.5
III	(a)	$(\kappa^5/2\pi)\int a^2 \sin^2\theta_a e^{-\kappa a}P_2(\cos\theta_b)[\Gamma_7/(\kappa b)^3]dv$	4.9	26.3	32.2	31.1	27.0	22.6	18.4	15.0
	(b)	$(\kappa^5/2\pi)\int a^2 \sin^2\theta_a e^{-\kappa a}P_2(\cos\theta_b)[\Gamma_7(\kappa b)/(\kappa b)^3 - (\kappa b)^2\Gamma_2(\kappa b)]dv$	−0.8	13.6	15.6	12.1	8.2	5.0	2.7	1.7
	(c)	$(\kappa^5/2\pi)\int a^2 \sin^2\theta_a e^{-\kappa a}P_2(\cos\theta_b)g_{7,3}dv$	5.7	12.7	16.6	19.0	18.8	17.6	15.7	13.3
IV	(a)	$(\kappa^5/2\pi)\int a^2 \cos^2\theta_a e^{-\kappa a}P_2(\cos\theta_b)[\Gamma_7/(\kappa b)^3]dv$	−91.4	−37.0	1.3	19.1	24.2	22.8	19.1	15.3
	(b)	$(\kappa^5/2\pi)\int a^2 \cos^2\theta_a e^{-\kappa a}P_2(\cos\theta_b)[\Gamma_7(\kappa b)/(\kappa b)^3 - (\kappa b)^2\Gamma_2(\kappa b)]dv$	−97.5	−44.0	−7.0	9.6	13.5	11.8	8.6	5.6
	(c)	$(\kappa^5/2\pi)\int a^2 \cos^2\theta_a e^{-\kappa a}P_2(\cos\theta_b)g_{7,3}dv$	6.1	7.0	8.3	9.5	10.7	11.0	10.5	9.7
V	(a)	$-(\kappa^5/2\pi)\int a^2 \sin\theta_a \cos\theta_a \sin\theta_b \cos\theta_b e^{-\kappa a}[\Gamma_7/(\kappa b)^3]dv$	38.0	42.1	34.4	24.7	16.7	11.0	7.2	4.7
	(b)	$-(\kappa^5/2\pi)\int a^2 \sin\theta_a \cos\theta_a \sin\theta_b \cos\theta_b e^{-\kappa a}[\Gamma_7/(\kappa b)^3 - g_{7,3}]dv$	41.6	41.5	31.6	20.6	12.4	7.0	3.8	2.0
	(c)	$-(\kappa^5/2\pi)\int a^2 \sin\theta_a \cos\theta_a \sin\theta_b \cos\theta_b e^{-\kappa a}g_{7,3}dv$	−3.6	0.6	2.8	4.1	4.3	4.0	3.4	2.7
VI	(a)	$(\kappa^5/2\pi)\int a^2 \sin^2\theta_a \sin^2\theta_b e^{-\kappa a}[\Gamma_7/(\kappa b)^3]dv$	229.	131.0	73.1	41.3	23.7	13.9	8.4	5.2
	(b)	$(\kappa^5/2\pi)\int a^2 \sin^2\theta_a \sin^2\theta_b e^{-\kappa a}[\Gamma_7/(\kappa b)^3 - g_{7,3}]dv$	190.9	100.0	49.9	24.5	11.7	5.5	2.6	1.2
	(c)	$(\kappa^5/2\pi)\int a^2 \sin^2\theta_a \sin^2\theta_b e^{-\kappa a}g_{7,3}dv$	38.1	31.0	23.2	16.8	12.0	8.4	5.8	4.0

$$i_1 = (\kappa/384)[Ic - (\tfrac{1}{5})\text{III}c]$$
$$i_3 = (\kappa/384)[Ic + (\tfrac{2}{5})\text{III}c] = (\kappa/192)[\text{II}c - (\tfrac{1}{5})\text{IV}c]$$
$$i_9 = (\kappa/192)[IIc + (\tfrac{2}{5})\text{IV}c]$$
$$i_5 = -\kappa\text{V}c/640 \quad i_7 = -\kappa\text{VI}c/1280$$

TABLE XIII

α	$\alpha=3$	4	5	6	7	8	9	10
i_1/κ	0.332	0.303	0.280	0.255	0.232	0.213	0.195	0.179
i_3/κ	.338	.324	.305	.285	.262	.241	.220	.200
i_9/κ	.359	.346	.332	.315	.296	.278	.252	.231
i_5/κ	−.0056	+.0009	+.0044	+.0064	+.0067	+.0062	+.0053	+.0042
i_7/κ	−.0312	−.0242	−.0181	−.0131	−.0094	−.0066	−.0045	−.0031

$$I_1 = 2\kappa/\alpha - 4c_1^2 \int e^{-\kappa a} a^2 \sin^2\theta_a(1/\kappa b)dv = \kappa[2/\alpha + i_1/\kappa - (\text{I}a)/192]$$

$$I_3 = 2\kappa/\alpha - 2\int dva_0^2/b - 2\int dva_1^2/b + i_3 = \kappa[2/\alpha + i_3/\kappa - (\text{II}a)/192 - (\text{I}a)/384]$$

$$I_9 = 2\kappa/\alpha - 4\int dva_0^2/b + i_9 = \kappa[2/\alpha + i_9/\kappa - (\text{II}a)/96]$$

$$I_5 = i_5,\ I_7 = i_7,\ I_6 = i_6,\ I_8 = i_8,\ I_{11} = i_{11} \cong -i_6$$

$$I_2 = 2\kappa S_{11}/\alpha - 4(S_{11})^{1/2}\int dva_1b_1/b + i_2$$

$$I_4 = 2\kappa S_{10}/\alpha - 2(S_{00})^{1/2}\int dva_1b_1/b - 2(S_{11})^{1/2}\int dva_0b_0/b + i_4$$

$$I_{10} = 2\kappa S_{00}/\alpha - 4(S_{00})^{1/2}\int dva_0b_0/b + i_{10}$$

The resulting integrals, after the small quantities before mentioned have been neglected, are listed in Table XIV. The relative energies are given in Table XV, and plotted in Fig. 1.

TABLE XIV. *Integrals.*

α	$\alpha=3$	4	5	6	7	8	9	10
I_1/κ	0.196	0.088	0.047	0.025	0.013	0.009	0.005	0.003
I_3/κ	.068	−.026	−.046	−.042	−.032	−.021	−.014	−.010
I_9/κ	−.043	−.140	−.140	−.110	−.067	−.042	−.026	−.013
I_5/κ	−.006	+.0007	.0044	.0064	.0067	.0062	.0053	.0042
I_7/κ	−.031	−.0240	−.0181	−.0131	−.0094	−.0066	−.0045	−.0031
I_2/κ	.082	.005	−.0217	−.0183	−.0139	−.0086	−.006	−.0028
I_4/κ	.074	.009	.0198	.0173	.0161	.0126	.0103	.0060
I_{10}/κ	.096	.070	.035	.032	.017	.0081	.0035	.0021
I_6/κ	−.043	−.030	−.039	−.028	−.021	−.015	−.010	−.006
I_8/κ		.01	.01	.007	.005			

TABLE XV. *Relative energies.*

α	$\alpha=3$	4	5	6	7	8	9	10
${}^3\Sigma_u{}^+/\kappa$		.100	.064	.032	.015			
${}^3\Delta_u/\kappa$	.329	.162	.103	.056	.032	.019	.0118	.0062
${}^1\Sigma_u{}^-/\kappa$		.225	.142	.081	.048			
${}^3\Sigma_g{}^-/\kappa$		.074	.026	.012	.003			
${}^1\Delta_g/\kappa$	.167	.063	.0188	.006	−.001	−.001	−.001	0
${}^1\Sigma_g{}^+/\kappa$		.053	.011	−.0005	−.0042			
${}^3\Pi_g/\kappa$	.137	.010	.009	−.003	−.002			
${}^3\Pi_u/\kappa$	.05	−.002	−.027	−.024	−.018	−.012	−.009	−.006
${}^1\Pi_g/\kappa$	.065	−.042	−.059	−.053	−.033	−.019	−.010	−.006
${}^1\Pi_u/\kappa$	−.06	−.076	−.110	−.087	−.069	−.050	−.037	−.025
${}^1\Sigma_g{}^+/\kappa$	.04	−.07	−.11	−.079	−.054	−.036	−.023	−.011
${}^3\Sigma_u{}^+/\kappa$	−.18	−.22	−.177	−.146	−.102	−.057	−.033	−.017

DISCUSSION

Fig. 1 shows the relative energies plotted as a function of the internuclear distance. The lowest term,[8] for intermediate values of κR, is the ${}^3\Sigma_u{}^+$. For hydrogen, we may set $\kappa=1$, and the minimum of this curve lies at about 2.0A. The value of the heat of dissociation is 2.9 volts, approximately.

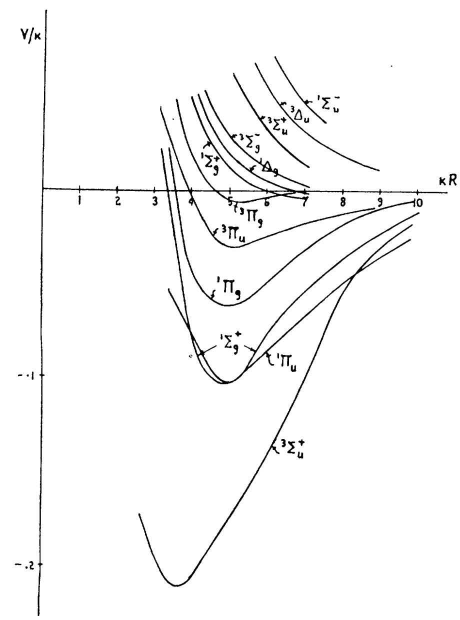

Fig. 1. Relative energies.

It is not possible to say, to the degree of approximation used here, whether the ${}^3\Pi_g$ state has a weak minimum or is repulsive. For the same reason, the relative positions of ${}^1\Sigma_g{}^+$ and ${}^1\Pi_u$ may actually be somewhat different. The

[8] This result has been predicted for B_2 by J. E. Lennard-Jones, Trans. Faraday Soc. **25**, 681 (1929).

reason for this uncertainty lies partly in the fact that we have neglected $i_6^{(3)}$ and $i_6^{(4)}$, and partly in the low degree of accuracy to which s_2 may be given.

Apart from these minor details, it is safe to assert that the curves do represent the interaction of two hydrogen-like atoms, each with one $2p$ electron, insofar as this interaction is to be found by a first order perturbation calculation of the Kemble and Zener type.

Heisenberg[9] has shown that there is reason to believe that the behavior of ferromagnetic substances may some day be understood, when it becomes possible to carry through detailed calculations. A necessary condition for ferromagnetism seems to be that the exchange integral for the lowest states be positive. This was found to be likely for $n \geqq 3$, where n is the principal quantum number. From our results, it is seen that a positive exchange energy integral is obtained for $n=2$, $l=1$, so that the possibility of ferromagnetism does not seem to be governed by the principal quantum number in so simple a fashion. The sufficient conditions for ferromagnetism have yet to be given.

One also sees from the curves in the figure that the "Coulomb" integrals are in general more important than the "exchange" integrals. The states arising from $m_{la}=0$, $m_{lb}=0$ lie the lowest, those from $m_{la}=0$, $m_{lb}=\pm 1$ are next higher, and those from $m_{la}=\pm 1$, $m_{lb}=\pm 1$ are highest. This means that the most stable configuration is that in which there is the maximum overlapping of charge, in accordance with the ideas of Slater[10] on directed valency. Orbital valency may be associated with the "Coulomb" integrals, and spin valency with the exchange integrals. The latter concept may, however, be misleading.

Though this analysis is strictly applicable only to the case where two excited hydrogen atoms interact (leaving out of account the influence of the s orbits) one might expect that similar conditions would obtain for boron, or excited lithium. Unfortunately, the band spectrum of B_2 has not been analyzed, so that a direct check of the theory is wanting. The inner s electrons would probably have some influence, but whether the order of the energy levels would be affected or not is open to question.

In conclusion, I wish to express may deep appreciation to the many people with whom the problem has been discussed. It was suggested by Professor Heisenberg, whom I also wish to thank for his help on previous problems. Acknowledgment must also be made to Dr. Dirac for discussion of allied problems. The work was continued at the Eigenössische Technische Hochschule, Zürich, and completed in Urbana. Thanks are due Mr. W. H. Furry for assistance in checking part of the calculations.

Note added to proof, Feb. 17, 1931: The influence of the inner $2s$ electrons is now being studied, and will be made the subject of a later paper.

[9] W. Heisenberg, Zeits. f. Physik **49**, 619 (1928).
[10] J. C. Slater, American Physical Society meeting, Dec. 29, 1930, paper 17.