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WAVE FUNCTIONS OF THE HYDROGEN MOLECULAR ION

By D. R. BATES, KATHLEEN LEDSHAM and A. L. STEWART

Queen's University, Belfast, and University College, London

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CONTENTS

The $1s\sigma_g$, $2s\sigma_g$, $3s\sigma_g$, $2p\sigma_u$, $3p\sigma_u$, $4p\sigma_u$, $3d\sigma_g$, $4f\sigma_u$, $2p\pi_u$ and $3d\pi_g$ states of the hydrogen molecular ion are investigated. The main results are given in the form of tables of parameters from which the electronic wave functions (in spheroidal co-ordinates) can be obtained. A representative selection of contour diagrams is also presented.

1. The structure of the hydrogen molecular ion has been studied by a number of theorists; thus, Burrau (1927), Hylleraas (1931), Jaffé (1934), Sandeman (1935) and Johnson (1941) have solved the exact wave equation for the ground state; and Guillemin & Zener (1929), Morse & Stueckelberg (1929), Teller (1930), Dickinson (1933), Gilbert (1933), Coulson (1937), Pritchard & Skinner (1951) and others have performed approximate calculations on both this state and some of the excited states. However, in spite of this, adequate tables of the electronic wave functions do not appear to have been published. A demand for tables of these wave functions arose recently in connexion with investigations which are being undertaken in Belfast and London on a variety of problems, including the determination of such quantities as the oscillator strengths of the allowed and forbidden transitions of H_2^+, and the cross-sections associated with the excitation of hydrogen atoms by slow protons. It was necessary, therefore, to carry out the relevant computations. The present paper gives the results obtained for the following states:

united atom designation	separated atoms† designation	form of potential energy curve
$1s\sigma_g$	σ $(1s)$	deep minimum
$2s\sigma_g$	σ $(2s, 2p_z)$	repulsive
$3s\sigma_g$	σ $(3s, 3p_z, 3d_z)$	repulsive
$2p\sigma_u$	σ^* $(1s)$	repulsive
$3p\sigma_u$	σ^* $(2s, 2p_z)$	repulsive
$4p\sigma_u$	σ^* $(3s, 3p_z, 3d_z)$	repulsive
$3d\sigma_g$	σ $(2s, 2p_z)$	shallow minimum
$4f\sigma_u$	σ^* $(2s, 2p_z)$	repulsive
$2p\pi_u$	π $(2p_x)$	shallow minimum
$3d\pi_g$	π^* $(2p_x)$	repulsive

In the case of H_2^+ the united atom designation is especially appropriate (cf. Herzberg 1950), and consequently the separated atoms designation (which though convenient in chemical discussions is sometimes ambiguous) is not used hereafter. As a wide range of inter-nuclear separations is covered the actual wave functions would occupy very many pages. Instead of displaying them in full, sets of parameters are tabulated from which they may readily be derived.

2. Ignoring the finiteness of the mass of the protons the Schrödinger equation for the electronic wave functions of H_2^+ is

$$\frac{\partial}{\partial\lambda}\left\{(\lambda^2-1)\frac{\partial\Psi}{\partial\lambda}\right\}+\frac{\partial}{\partial\mu}\left\{(1-\mu^2)\frac{\partial\Psi}{\partial\mu}\right\}+\left\{\frac{1}{\lambda^2-1}+\frac{1}{1-\mu^2}\right\}\frac{\partial^2\Psi}{\partial\phi^2}+\{\tfrac{1}{4}R^2E(\lambda^2-\mu^2)+2R\lambda\}\Psi=0, \quad (1)$$

where λ and μ are the usual confocal elliptic co-ordinates, ϕ is the azimuthal angle, R is the distance between the two nuclei in atomic units, and E is the electronic energy in Rydbergs. Writing

$$\Psi(\lambda,\mu,\phi)=\Lambda(\lambda)\,\mathrm{M}(\mu)\,\Phi(\phi) \quad (2)$$

and

$$p^2=-\tfrac{1}{4}R^2E, \quad (3)$$

we obtain at once (cf. Baber & Hassé 1935) that

$$\Phi(\phi)=\begin{matrix}\cos\\ \sin\end{matrix}(m\phi) \quad (m=0,1,2,\ldots), \quad (4)$$

and that $\mathrm{M}(\mu)$ and $\Lambda(\lambda)$ satisfy

$$\frac{\mathrm{d}}{\mathrm{d}\mu}\left\{(1-\mu^2)\frac{\mathrm{dM}}{\mathrm{d}\mu}\right\}+\left\{-A+p^2\mu^2-\frac{m^2}{1-\mu^2}\right\}\mathrm{M}=0 \quad (5)$$

and

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\left\{(\lambda^2-1)\frac{\mathrm{d}\Lambda}{\mathrm{d}\lambda}\right\}+\left\{A+2R\lambda-p^2\lambda^2-\frac{m^2}{\lambda^2-1}\right\}\Lambda=0, \quad (6)$$

A being a separation constant.

Equation (5) has been studied in great detail by Stratton, Morse, Chu & Hutner (1941). If m and p are specified, proper solutions exist only for particular values of the separation constant. These eigenvalues are the roots of an equation involving an infinite continued fraction. The eigenfunction, $\mathrm{M}(l,m,p\,|\,\mu)$, corresponding to the $(1-m+l)$th root, $A(l,m,p)$, may be expanded in terms of the associated Legendre polynomials,

$$\mathrm{M}(l,m,p\,|\,\mu)=\sum_s{}'f_s(l,m,p)\,P^m_{m+s}(\mu), \quad (7)$$

† The symbols within the brackets represent the atomic orbitals, which, of course, belong to both nuclei. Odd (u) states are indicated with an asterisk, and even (g) states are left plain (cf. Coulson 1952). The former are all unstable but the latter are *not* all stable.

the summation being over even values of s if $(l+m)$ is even, and over odd values of s if $(l+m)$ is odd. Stratton *et al.* have published tables giving the separation constants and the expansion coefficients as functions of p for the lower values of l and m (which are the values of most interest).

Analytical solutions of (6) have been derived by Jaffé (1934), who writes

$$\Lambda(\lambda) = (\lambda^2-1)^{\frac{1}{2}m}(\lambda+1)^{\sigma}\exp(-p\lambda)\,y(\zeta), \tag{8}$$

with
$$\sigma = \frac{R}{p} - m - 1, \tag{9}$$

and
$$\zeta = (\lambda-1)/(\lambda+1), \tag{10}$$

so that
$$\zeta(1-\zeta)^2\frac{\mathrm{d}^2y}{\mathrm{d}\zeta^2} + [-(m+2\sigma-1)\,\zeta^2 + 2(\sigma-2p-1)\,\zeta + m + 1]\frac{\mathrm{d}y}{\mathrm{d}\zeta}$$
$$+ [\sigma(\sigma+m)\,\zeta + \sigma(1+2p) + m(m+1+\sigma) + A']\,y = 0, \tag{11}$$

where
$$A' = A - p^2. \tag{12}$$

Taking
$$y = \sum_{t=0}^{\infty} g_t\zeta^t \tag{13}$$

and substituting in (11), he obtains the three-term recurrence relation

$$\alpha_t g_{t+1} - \beta_t g_t + \gamma_t g_{t-1} = 0, \tag{14}$$

with
$$\left.\begin{aligned} \alpha_t &= (t+1)\,(t+m+1),\\ \beta_t &= 2t^2 + (4p-2\sigma)\,t - A' - 2p\sigma - (m+1)\,(m+\sigma),\\ \gamma_t &= (t-1-\sigma)\,(t-1-\sigma-m). \end{aligned}\right\} \tag{15}$$

It follows that
$$g_t/g_{t-1} = F_t, \tag{16}$$
where F_t is the continued fraction

$$\frac{\gamma_t}{\beta_t} - \frac{\alpha_t\gamma_{t+1}}{\beta_{t+1}} - \frac{\alpha_{t+1}\gamma_{t+2}}{\beta_{t+2}} - \ldots. \tag{17}$$

Noting that g_{-1} is zero we have therefore that

$$\beta_0/\alpha_0 = F_1. \tag{18}$$

The eigenvalues of σ, for given p, m and A', are the roots of this equation. When p is zero they can be found by inspection, but in general it is necessary to proceed by successive approximations. The designation $\sigma(n, l, m; p)$ will be used to denote the $(n-l)$th root, the constant A' being taken as

$$A'(l, m; p) = A(l, m; p) - p^2. \tag{19}$$

Computations were carried out giving $\sigma(n, l, m; p)$ as a function of p for the following cases:

$$m = 0 \quad \begin{cases} l = 0;\ n = 1, 2, 3 & (\text{i.e. } 1s\sigma_g,\ 2s\sigma_g,\ 3s\sigma_g),\\ l = 1;\ n = 2, 3, 4 & (\text{i.e. } 2p\sigma_u,\ 3p\sigma_u,\ 4p\sigma_u),\\ l = 2;\ n = 3 & (\text{i.e. } 3d\sigma_g),\\ l = 3;\ n = 4 & (\text{i.e. } 4f\sigma_u), \end{cases}$$

$$m = 1 \quad \begin{cases} l = 1;\ n = 2 & (\text{i.e. } 2p\pi_u),\\ l = 2;\ n = 3 & (\text{i.e. } 3d\pi_g). \end{cases}$$

The corresponding values of the distance between the two protons, $R(n, l, m; p)$, were got from (9) and, with the aid of inverse interpolation, the basic parameters were then determined as functions of this distance. For the ten states studied we thus have $p(n, l, m; R)$ (and hence, from (3), $E(n, l, m; R)$), $A'(n, l, m; R)$ and $\sigma(n, l, m; R)$. Table 1 gives the values obtained.† An R-range of from 0 to 10 is covered where the data of Stratton *et al.* are sufficiently extensive to make this possible. Finally, the coefficients of the μ-expansion (which Stratton *et al.* present as $f(m, l; p)$) were converted to the form $f(n, l, m; R)$ by direct interpolation; and the coefficients of the λ-expansion, $g(n, l, m; R)$, were found by numerical substitution in Jaffé's recurrence relation. These coefficients are displayed in tables 2 and 3 respectively. Normalization factors are not included but they may easily be computed. It may be noted that the results can be modified to apply to the more general system in which the charges on the nuclei are Z instead of unity; all that is necessary is to multiply the R columns by Z^{-1} and the E columns by Z^2. The case $Z = 0{\cdot}5$ is artificial but nevertheless of some interest representing as it does the simplest conceivable neutral molecule.

TABLE 4. COMPARISON OF EXACT AND L.C.A.O. WAVE FUNCTIONS OF $1s\sigma_g$ AND $2p\sigma_u$ STATES OF THE HYDROGEN MOLECULAR ION

distance from centre along inter-nuclear axis (in atomic units)		wave function			wave function	
		exact	L.C.A.O.		exact	L.C.A.O.
0	$1s\sigma_g$ $R=2$	0·315	0·233	$1s\sigma_g$ $R=4$	0·127	0·099
1		0·458	0·360		0·175	0·153
2		0·120	0·132		0·378	0·373
3		0·030	0·049		0·123	0·137
4		0·007	0·018		0·039	0·050
0	$2p\sigma_u$ $R=2$	0·000	0·000	$2p\sigma_u$ $R=4$	0·000	0·000
1		0·453	0·536		0·146	0·141
2		0·199	0·197		0·436	0·435
3		0·078	0·073		0·158	0·160
4		0·029	0·027		0·055	0·059

In treating complex molecules frequent use is made of the L.C.A.O. approximation, so it is instructive to examine how accurate this is in the case of H_2^+. Table 4 shows a comparison with the two centre wave functions of the $1s\sigma_g$ and $2p\sigma_u$ states which, on the L.C.A.O. approximation, are represented by

$$[e^{-r_1} + e^{-r_2}]/[2\pi(1+S)]^{\frac{1}{2}} \tag{20}$$

and

$$[e^{-r_1} - e^{-r_2}]/[2\pi(1-S)]^{\frac{1}{2}} \tag{21}$$

respectively, r_1 and r_2 being the distances of the electron from the two nuclei and S being the function

$$(1 + R + \tfrac{1}{3}R^2)\, e^{-R}. \tag{22}$$

† A similar table giving the binding energy of an electron in the combined field of a proton and a negative meson was prepared some years ago but was not published owing to the appearance of a paper by Wightman (1950) which included an account of independent calculations on this binding energy. However, it is perhaps worth taking this opportunity of recording the check on Wightman's numerical results. (Tables 1, 2 and 3 are printed at the end of the paper.)

As can be seen the agreement is but moderate. It may be noted also in this connexion that the use of (20) and (21) in the calculation of the oscillator strength of the $1s\sigma_g$ to $2p\sigma_u$ transition does not yield very precise results (Bates 1951).

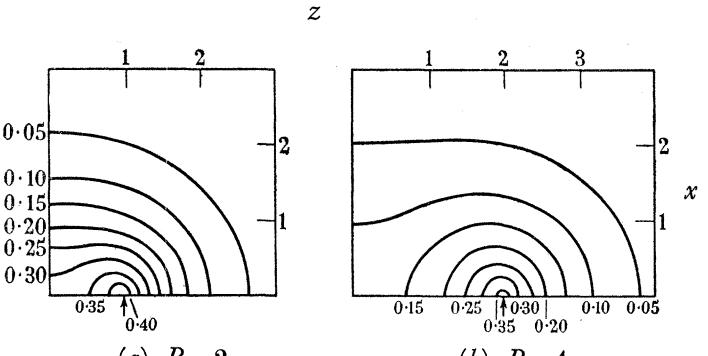
TABLE 5. COMPARISON OF THE EXACT AND L.C.A.O. POTENTIAL ENERGIES OF THE $2s\sigma_g$, $3p\sigma_u$, $3d\sigma_g$ AND $4f\sigma_u$ STATES OF THE HYDROGEN MOLECULAR ION

inter-nuclear separation R (atomic units)	potential energy $2/R+E$ (Rydbergs)							
	$2s\sigma_g$		$3p\sigma_u$		$3d\sigma_g$		$4f\sigma_u$	
	exact	L.C.A.O. approx.	exact	L.C.A.O. approx.	exact	L.C.A.O. approx.	exact	L.C.A.O. approx.
1	+1·154	+1·334	+1·521	+1·560	+1·550	+0·594	+1·749	+0·894
2	+0·278	+0·380	+0·489	+0·500	+0·528	−0·170	+0·747	−0·297
3	+0·029	+0·090	+0·160	+0·172	+0·152	−0·324	+0·409	−0·668
4	−0·077	−0·037	+0·010	+0·020	−0·071	−0·364	+0·235	−0·806
6	−0·162	−0·141	−0·122	−0·115	−0·292	−0·372	+0·041	−0·745
8	−0·194	−0·182	−0·175	−0·170	−0·347	−0·360	−0·085	−0·344
10	−0·209	−0·203	−0·201	−0·198	−0·346	−0·343	−0·170	−0·207
∞	−0·250	−0·250	−0·250	−0·250	−0·250	−0·250	−0·250	−0·250

For the other states it was found, on making a similar comparison to that in table 4, that the L.C.A.O. approximation† is in the main poor, as of course would be expected since the atomic orbitals involved are excited. Instead of displaying this comparison, table 5 is presented as being perhaps of more interest to chemists. It gives the exact and approximate values of the potential energies of several of the states. Clearly, the difference between them is sometimes considerable even at quite large inter-nuclear separations. The matter will not be pursued further in the present paper as a more detailed assessment of the L.C.A.O. and other approximations will be published elsewhere.

A number of contour diagrams (figures 1 to 8) are given to illustrate the general form of the H_2^+ wave functions. In these the normalization is as usual; the origin of the co-ordinate system is at the centre of the ion; the position of one proton is marked by a small arrow; the z-axis is along the inter-nuclear line; and the x-axis is perpendicular to this line and (in the case of π states) to the nodal plane.

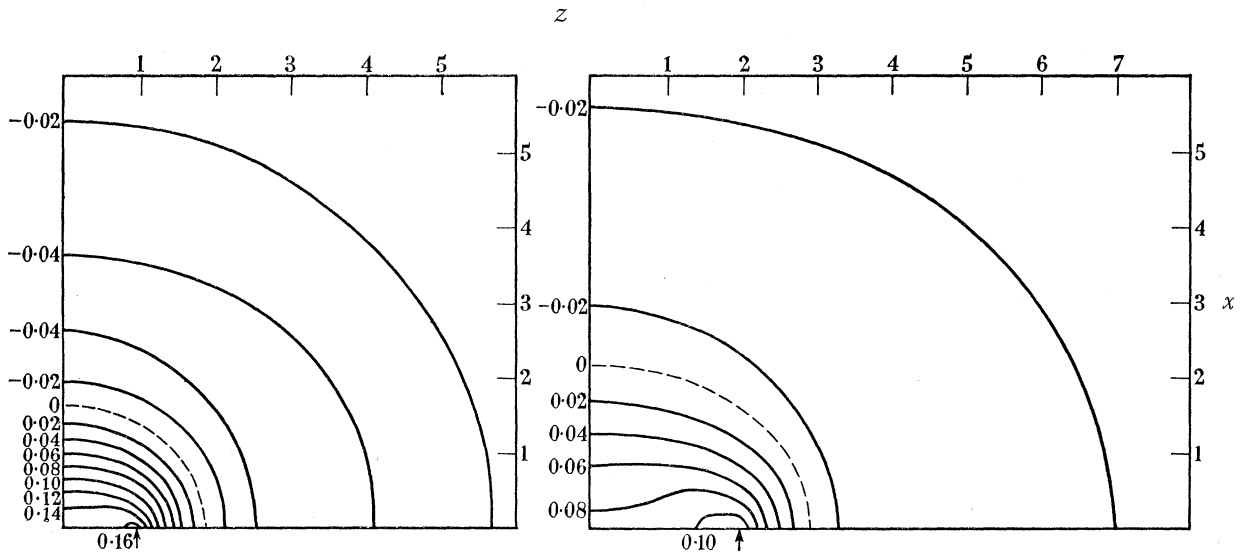
FIGURES 1 TO 8. Contour diagrams of normalized wave functions of H_2^+.



(a) $R=2$ (b) $R=4$

FIGURE 1. $1s\sigma_g$

† The σ states were treated (cf. Gilbert 1933) as hybrids of the $2s$ and $2p_z$ atomic states or of the $3s$, $3p_z$ and $3d_z$ atomic states; the π states were based on only the $2p_x$ atomic state.



(*a*) $R = 2$ (*b*) $R = 4$

FIGURE 2. $2s\sigma_g$.

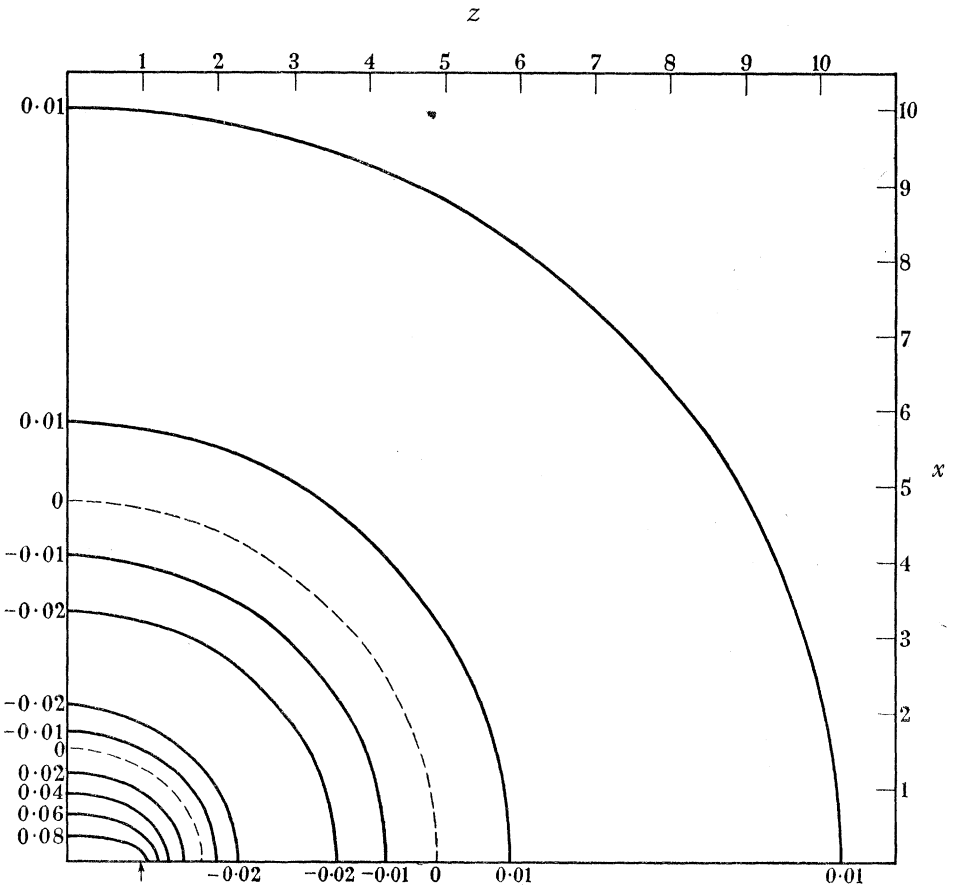


FIGURE 3 (*a*). $3s\sigma_g$, $R = 2$.

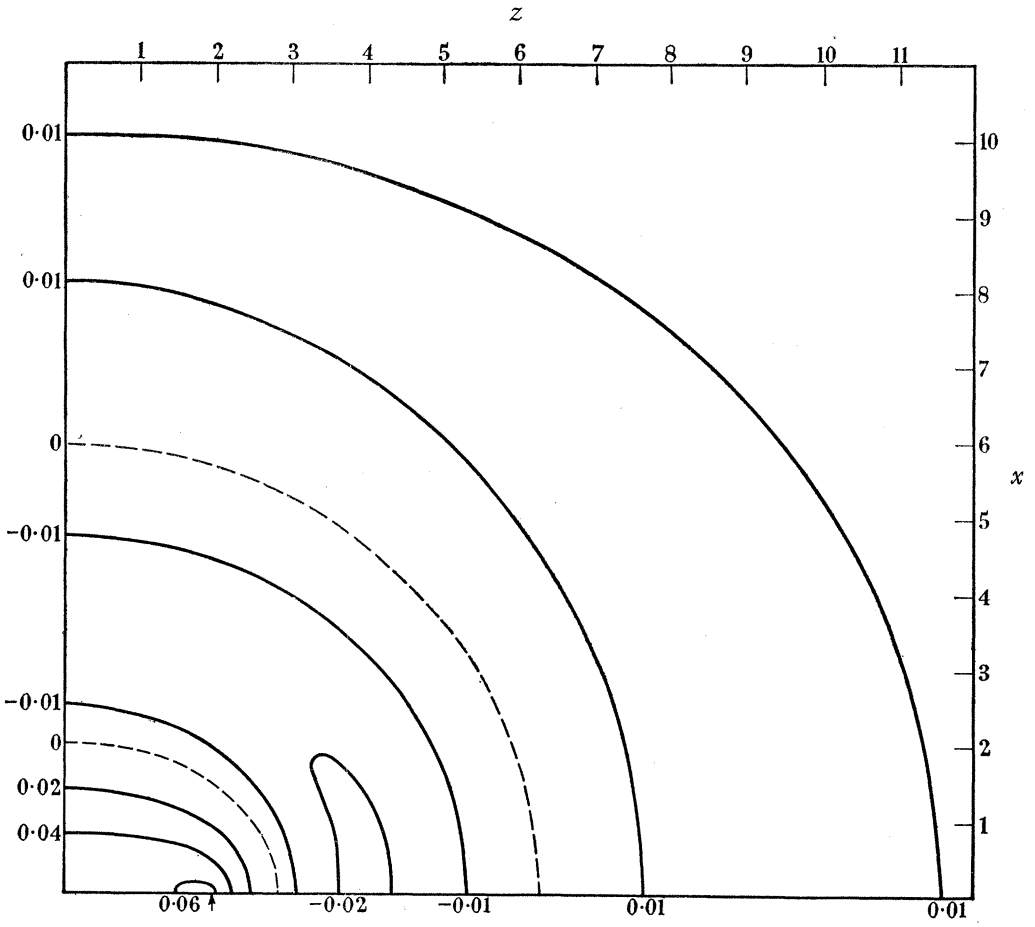
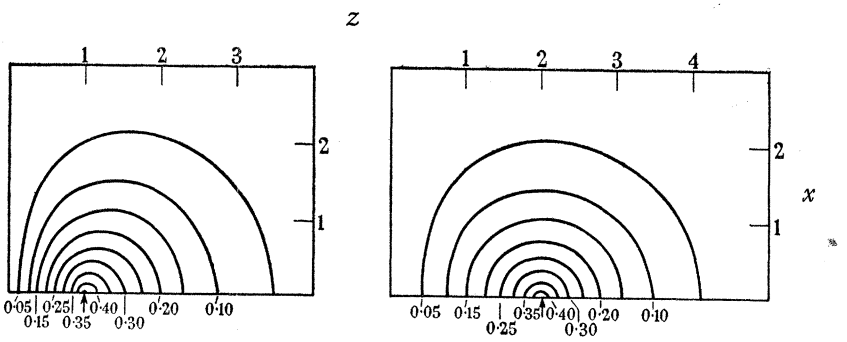
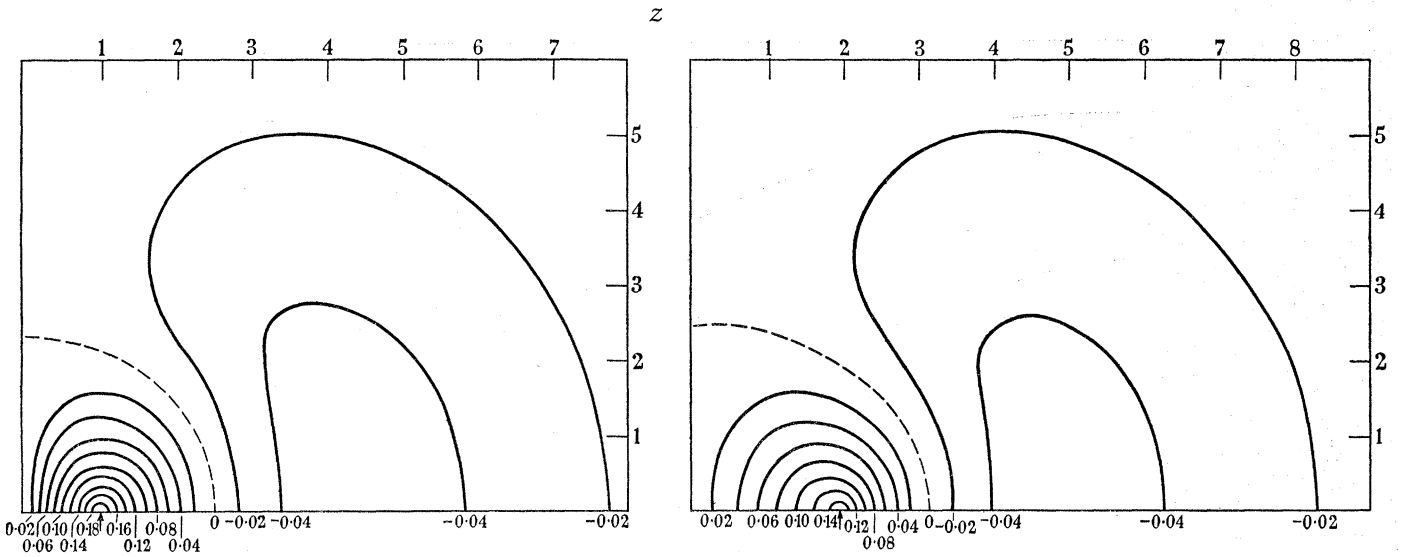


FIGURE 3 (*b*). $3s\sigma_g$, $R = 4$.



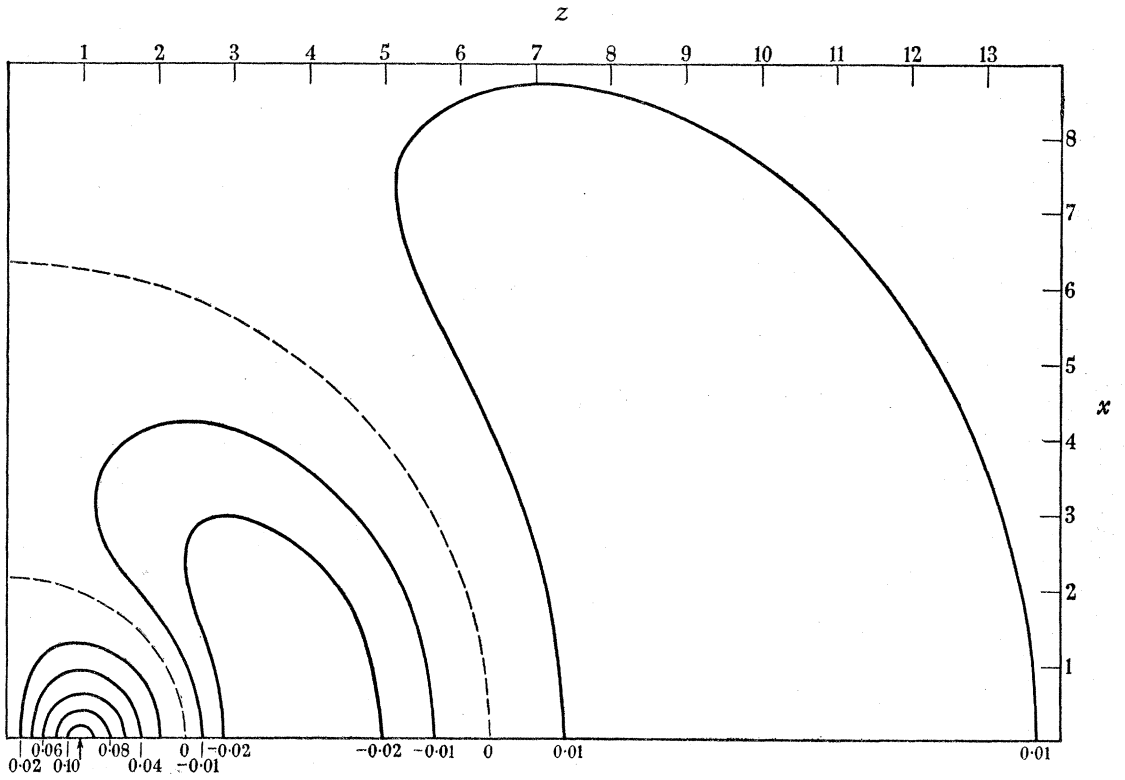
(*a*) $R = 2$ (*b*) $R = 4$

FIGURE 4. $2p\sigma_u$.



(*a*) $R=2$ (*b*) $R=4$

FIGURE 5. $3p\sigma_u$.



(*a*) $R=2$

FIGURE 6. $4p\sigma_u$.

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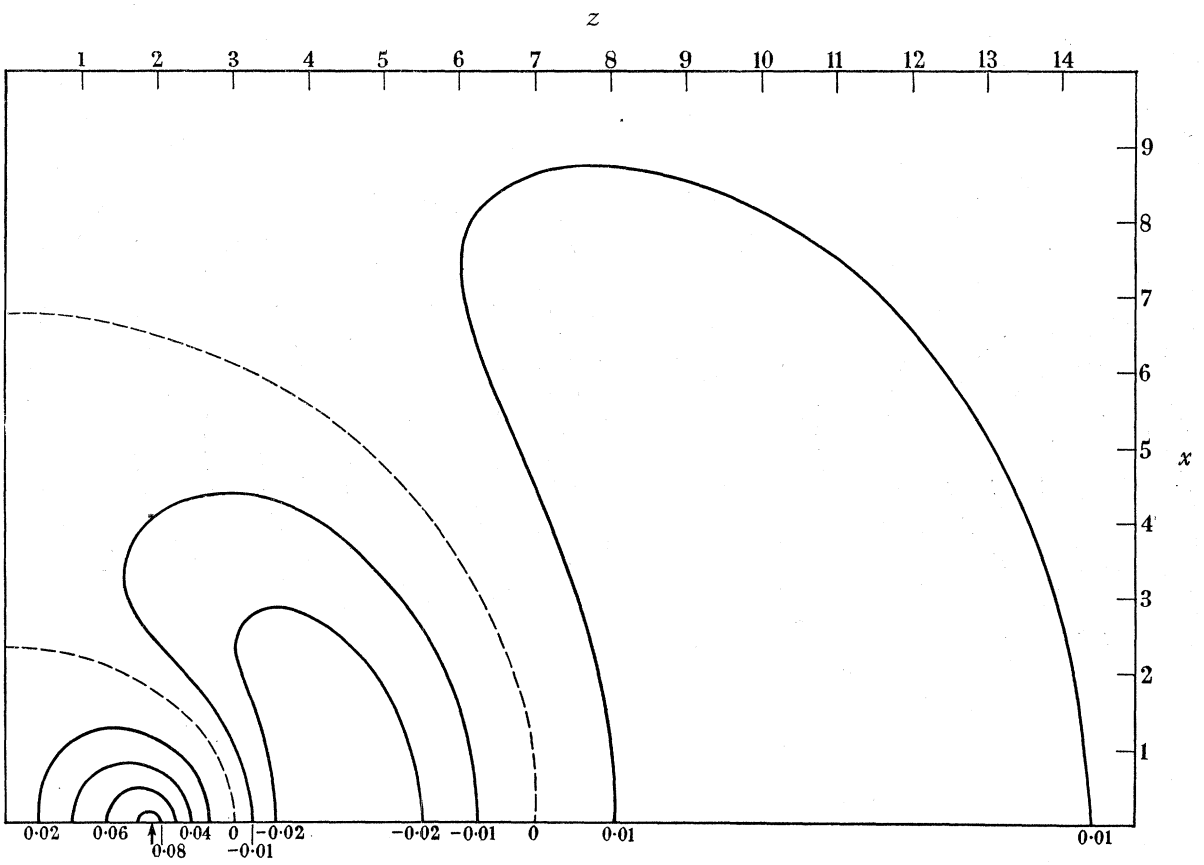
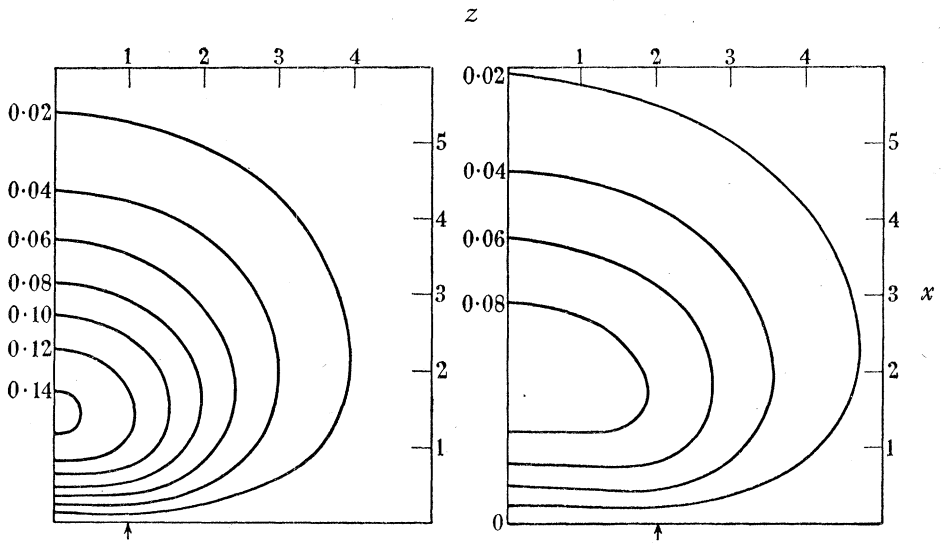


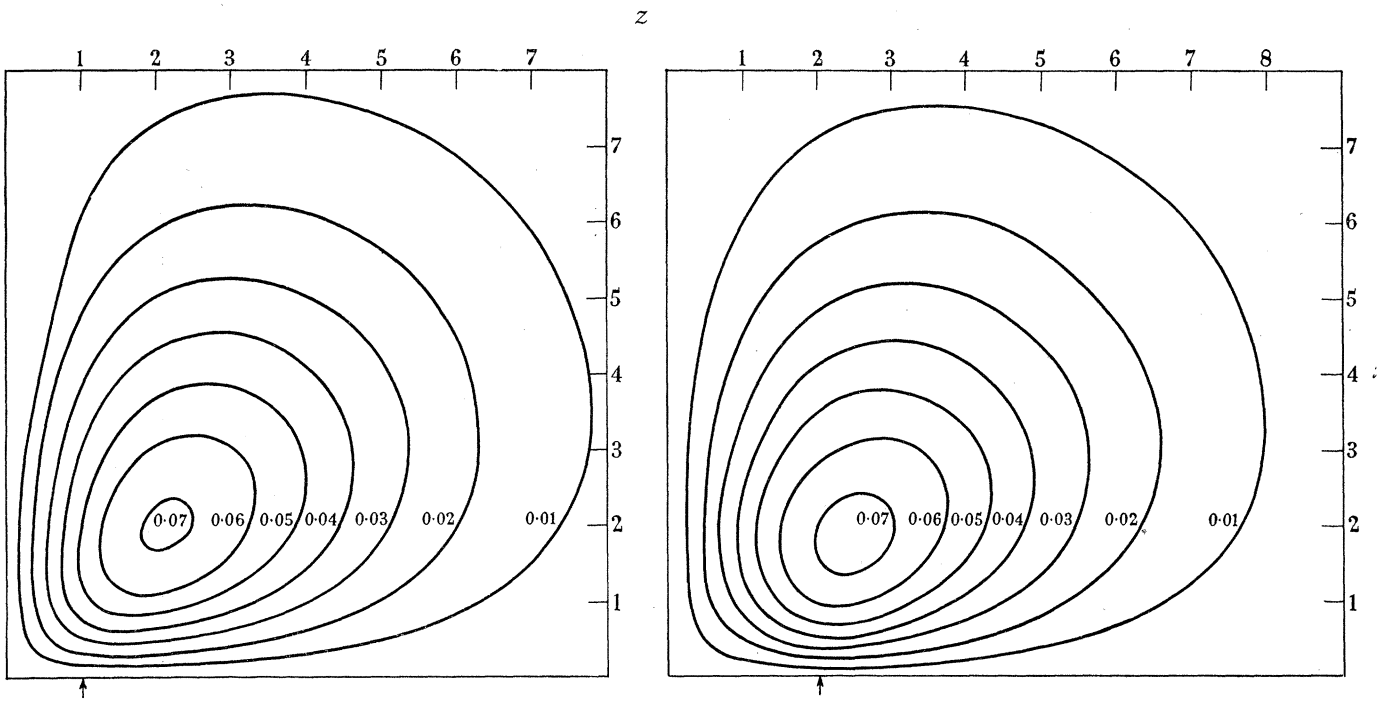
(*b*) $R = 4$

FIGURE 6. $4p\sigma_u$.



(*a*) $R = 2$ (*b*) $R = 4$

FIGURE 7. $2p\pi_u$.



(*a*) $R=2$ (*b*) $R=4$

FIGURE 8. $3d\pi_g$.

In conclusion, we wish to thank Professor H. S. W. Massey, F.R.S., for the encouragement he gave us during the course of the calculations.

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NOTE ON THE TABLES

Though the figures in the three groups of tables are generally correct to the last decimal place retained some are certainly in error by one unit, and there is the possibility that a few are in error by several units; little significance can be attached to the last decimal place of the bracketed figures.

Casual inspection of tables 3 might suggest that some of the g_t series should have been carried further. This is not the case; these series finally converge extremely rapidly and the higher members (for which values are not presented) may be neglected.

Derived wave functions should be accurate to at least 1 part in 5000 over the main part of their range. Moreover, as the smaller f_s coefficients are given to extra decimal places, computational difficulties should not occur in applications in which the usual dominance of the contribution from the larger coefficients is reduced by effects arising from the orthogonal properties of the associated Legendre polynomials.

Throughout, the internuclear separation, R, is in units of a_0, the radius of the first Bohr orbit, and the energy is in Rydbergs.

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TABLE 1. THE BASIC PARAMETERS

	$1s\sigma_g$				$2s\sigma_g$				
R	p	σ	$-A'$	$-E$	R	p	σ	$-A'$	$-E$
0·0	0·00000	0·00000	0·00000	4·00000	**0·0**	0·00000	1·00000	0·00000	1·00000
0·2	0·19640	0·01831	0·02569	(3·85741)	**0·2**	0·09909	(1·01832)	0·00654	(0·98193)
0·4	0·37956	0·05386	0·09573	(3·60157)	**0·4**	0·19475	(1·05392)	0·02526	(0·94819)
0·6	0·54852	0·09386	0·19923	(3·34301)	**0·6**	0·28653	(1·09399)	0·05464	(0·91224)
0·8	0·70529	0·13429	0·32790	(3·10895)	**0·8**	0·37476	1·13471	0·09333	0·87777
1·0	0·85199	0·17372	0·47595	(2·90356)	**1·0**	0·45985	1·17462	0·14030	0·84585
1·2	0·99038	0·21165	0·63923	(2·72461)	**1·2**	0·54218	1·21327	0·19468	0·81657
1·4	1·12186	0·24792	0·81469	(2·56853)	**1·4**	0·62208	1·25053	0·25574	0·78975
1·6	1·24755	0·28251	1·00004	(2·43186)	**1·6**	0·69979	1·28639	0·32287	0·76517
1·8	1·36836	0·31545	1·19346	(2·31162)	**1·8**	0·77555	1·32092	0·39553	0·74257
2·0	1·48501	0·34679	1·39352	2·20525	**2·0**	0·84954	1·35420	0·47326	0·72173
2·2	1·59813	0·37661	1·59905	2·11076	**2·2**	0·92193	1·38630	0·55565	0·70244
2·4	1·70823	0·40496	1·80905	2·02642	**2·4**	0·99284	1·41730	0·64233	0·68454
2·6	1·81577	0·43190	2·02267	1·95090	**2·6**	1·06241	1·44727	0·73295	0·66788
2·8	1·92111	0·45749	2·23921	1·88299	**2·8**	1·13073	1·47627	0·82721	0·65232
3·0	2·02460	0·48177	2·45803	1·82178	**3·0**	1·19791	1·50436	0·92483	0·63777
3·2	2·12654	0·50479	2·67857	1·76647	**3·2**	1·26402	1·53160	1·02554	0·62412
3·4	2·22719	0·52659	2·90035	1·71639	**3·4**	1·32915	1·55803	1·12910	0·61129
3·6	2·32679	0·54720	3·12294	1·67097	**3·6**	1·39335	1·58370	1·23527	0·59921
3·8	2·42554	0·56666	3·34597	1·62971	**3·8**	1·45670	1·60863	1·34383	0·58780
4·0	2·52362	0·58502	3·56909	1·59216	**4·0**	1·51925	1·63287	1·45459	0·57703
4·2	2·62121	0·60231	3·79201	1·55799	**4·2**	1·58106	1·65645	1·56735	0·56684
4·4	2·71845	0·61857	4·01451	1·52685	**4·4**	1·64217	1·67939	1·68192	0·55717
4·6	2·81545	0·63384	4·23637	1·49844	**4·6**	1·70263	1·70171	1·79813	0·54801
4·8	2·91234	0·64816	4·45743	1·47252	**4·8**	1·76248	1·72344	1·91581	0·53929
5·0	3·00919	0·66157	4·67756	1·44884	**5·0**	1·82176	1·74460	2·03482	0·53101
5·5	3·25164	0·69145	5·22323	1·39810	**5·5**	1·96774	1·79509	2·33710	0·51200
6·0	3·49505	0·71671	5·76182	1·35726	**6·0**	2·11092	1·84236	2·64448	0·49511
6·5	3·73979	0·73807	6·29359	1·32412	**6·5**	2·25177	1·88662	2·95501	0·48004
7·0	3·98585	0·75621	6·81922	1·29690	**7·0**	2·39068	1·92804	3·26701	0·46656
7·5	4·23311	0·77175	7·33975	1·27426	**7·5**	2·52799	1·96679	3·57904	0·45445
8·0	4·48133	0·78519	7·85608	1·25514	**8·0**	2·66399	2·00301	3·88990	0·44355
8·5	4·73028	0·79693	8·36915	1·23878	**8·5**	2·79894	2·03686	4·19864	0·43372
9·0	4·97979	0·80730	8·87974	1·22461	**9·0**	2·93304	2·06849	4·50456	0·42483
					9·5	3·06645	2·09805	4·80717	0·41676
					10·0	3·19930	2·12568	5·10618	0·40942

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

$3s\sigma_g$

R	p	σ	$-A'$	$-E$
0·0	0·00000	2·0000	0·00000	0·44444
0·2	0·06626	2·0183	0·00293	(0·43905)
0·4	0·13098	2·0539	0·01143	(0·42891)
0·6	0·19392	2·0940	0·02505	(0·41783)
0·8	0·25521	2·1347	0·04336	(0·40706)
1·0	0·314988	2·17472	0·06600	0·39687
1·2	0·373433	2·21343	0·09267	0·38737
1·4	0·430664	2·25079	0·12313	0·37851
1·6	0·486795	2·28680	0·15714	0·37026
1·8	0·541922	2·32151	0·19449	0·36257
2·0	0·596123	2·35501	0·23502	0·35536
2·2	0·649467	2·38739	0·27854	0·34860
2·4	0·702014	2·41873	0·32490	0·34224
2·6	0·753818	2·44911	0·37397	0·33624
2·8	0·804926	2·47858	0·42560	0·33056
3·0	0·855382	2·50721	0·47968	0·32519
3·2	0·905220	2·53505	0·53609	0·32009
3·4	0·954478	2·56216	0·59471	0·31523
3·6	1·003183	2·58858	0·65545	0·31061
3·8	1·051366	2·61434	0·71821	0·30620
4·0	1·099053	2·63950	0·78287	0·30198
4·2	1·146266	2·66407	0·84936	0·29794
4·4	1·193030	2·68809	0·91758	0·29407
4·6	1·239363	2·71158	0·98745	0·29036
4·8	1·285286	2·73458	1·05889	0·28680
5·0	1·330818	2·75709	1·13181	0·28337
5·5	1·443035	2·81141	1·32010	0·27535
6·0	1·553141	2·86314	1·51602	0·26803
6·5	1·661349	2·91248	1·71849	0·26131
7·0	1·767842	2·95963	1·92649	0·25512
7·5	1·872790	3·00472	2·13905	0·24941
8·0	1·976338	3·04789	2·35529	0·24412
8·5	2·078625	3·08924	2·57434	0·23921
9·0	2·179774	3·12887	2·79541	0·23464
9·5	2·279896	3·16686	3·01780	0·23038
10·0	2·379092	3·20328	3·24083	0·22640

$2p\sigma_u$

R	p	σ	$-A'$	$-E$
0·0	0·00000	1·00000	2·00000	1·00000
0·2	0·10027	(0·99467)	2·00402	(1·00535)
0·4	0·20215	(0·97877)	2·01633	(1·02158)
0·6	0·30720	0·95309	2·03769	1·04861
0·8	0·41675	0·91963	2·06927	1·08548
1·0	0·53142	0·88175	2·11241	1·12962
1·2	0·65100	0·84332	2·16829	1·17722
1·4	0·77449	0·80764	2·23748	1·22415
1·6	0·90056	0·77666	2·31993	1·26721
1·8	1·02792	0·75111	2·41507	1·30446
2·0	1·15545	0·73092	2·52196	1·33507
2·2	1·28239	0·71554	2·63955	1·35912
2·4	1·40823	0·70427	2·76678	1·37715
2·6	1·53263	0·69643	2·90261	1·38991
2·8	1·65545	0·69138	3·04610	1·39822
3·0	1·77663	0·68859	3·19639	1·40285
3·2	1·89614	0·68764	3·35271	1·40443
3·4	2·01404	0·68815	3·51439	1·40358
3·6	2·13041	0·68981	3·68083	1·40082
3·8	2·24533	0·69240	3·85150	1·39654
4·0	2·35890	0·69571	4·02594	1·39110
4·2	2·47121	0·69958	4·20371	1·38478
4·4	2·58234	0·70388	4·38444	1·37779
4·6	2·69240	0·70851	4·56781	1·37032
4·8	2·80148	0·71338	4·75351	1·36255
5·0	2·90966	0·71841	4·94128	1·35458
5·5	3·17669	0·73136	5·41823	1·33439
6·0	3·43971	0·74434	5·90366	1·31462
6·5	3·69960	0·75695	6·39517	1·29581
7·0	3·95710	0·76897	6·89099	1·27826
7·5	4·21280	0·78029	7·38984	1·26206
8·0	4·46715	0·79086	7·89072	1·24721
8·5	4·72047	0·80067	8·39286	1·23365
9·0	4·97308	0·80974	8·89588	1·22131

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

TABLE 1. THE BASIC PARAMETERS (*cont.*)

	$3p\,\sigma_u$				$4p\,\sigma_u$				
R	p	σ	$-A'$	$-E$	R	p	σ	$-A'$	$-E$
0·0	0·00000	2·0000	2·00000	0·44444	**0·0**	0·00000	3·0000	2·00000	0·25000
0·2	(0·06679)	(1·9947)	2·00178	(0·44603)	**0·2**	(0·05007)	(2·9947)	2·00100	(0·25067)
0·4	0·13429	1·9790	2·00721	(0·45081)	**0·4**	(0·10053)	(2·9791)	2·00404	(0·25264)
0·6	0·20310	1·9542	2·01649	(0·45832)	**0·6**	0·15172	2·9546	2·00920	(0·25577)
0·8	0·273656	1·92338	2·02992	0·46805	**0·8**	0·20384	2·9247	2·01661	(0·25969)
1·0	0·345911	1·89092	2·04777	0·47862	**1·0**	0·25682	2·8937	2·02635	0·26383
1·2	0·419451	1·86088	2·07017	0·48872	**1·2**	0·31039	2·8661	2·03847	0·26762
1·4	0·493633	1·83612	2·09706	0·49729	**1·4**	0·364171	2·84435	2·05293	0·27065
1·6	0·567833	1·81773	2·12826	0·50380	**1·6**	0·417840	2·82922	2·06963	0·27280
1·8	0·641619	1·80540	2·16351	0·50824	**1·8**	0·471174	2·82024	2·08846	0·27408
2·0	0·714721	1·79829	2·20255	0·51083	**2·0**	0·524049	2·81644	2·10933	0·27463
2·2	0·786997	1·79543	2·24513	0·51187	**2·2**	0·576401	2·81679	2·13214	0·27458
2·4	0·858395	1·79592	2·29104	0·51170	**2·4**	0·628211	2·82037	2·15679	0·27406
2·6	0·928913	1·79897	2·34009	0·51058	**2·6**	0·679484	2·82643	2·18322	0·27319
2·8	0·998567	1·80402	2·39210	0·50874	**2·8**	0·730234	2·83439	2·21136	0·27206
3·0	1·067384	1·81061	2·44692	0·50636	**3·0**	0·780481	2·84378	2·24113	0·27073
3·2	1·135403	1·81838	2·50439	0·50357	**3·2**	0·830245	2·85428	2·27249	0·26926
3·4	1·202667	1·82705	2·56441	0·50049	**3·4**	0·879546	2·86563	2·30537	0·26768
3·6	1·269219	1·83639	2·62684	0·49720	**3·6**	0·928405	2·87762	2·33973	0·26603
3·8	1·335090	1·84625	2·69157	0·49376	**3·8**	0·976843	2·89008	2·37550	0·26433
4·0	1·400315	1·85650	2·75848	0·49022	**4·0**	1·024880	2·90290	2·41266	0·26259
4·2	1·464926	1·86704	2·82748	0·48662	**4·2**	1·072534	2·91596	2·45115	0·26085
4·4	1·528955	1·87778	2·89846	0·48300	**4·4**	1·119817	2·92921	2·49094	0·25909
4·6	1·592428	1·88867	2·97133	0·47936	**4·6**	1·166749	2·94258	2·53197	0·25734
4·8	1·655376	1·89964	3·04600	0·47574	**4·8**	1·213341	2·95602	2·57421	0·25559
5·0	1·717820	1·91067	3·12239	0·47214	**5·0**	1·259606	2·96949	2·61764	0·25386
5·5	1·871892	1·93820	3·32036	0·46334	**5·5**	1·373923	3·00314	2·73107	0·24961
6·0	2·023307	1·96544	3·52740	0·45486	**6·0**	1·486451	3·03646	2·85105	0·24550
6·5	2·172349	1·99215	3·74241	0·44678	**6·5**	1·597340	3·06926	2·97707	0·24156
7·0	2·319263	2·01820	3·96443	0·43910	**7·0**	1·706725	3·10142	3·10866	0·23779
7·5	2·464273	2·04349	4·19259	0·43183	**7·5**	1·814721	3·13287	3·24536	0·23418
8·0	2·607578	2·06798	4·42612	0·42497	**8·0**	1·921430	3·16357	3·38678	0·23074
8·5	2·749348	2·09164	4·66428	0·41849	**8·5**	2·026945	3·19350	3·53252	0·22746
9·0	2·889735	2·11447	4·90643	0·41237	**9·0**	2·131352	3·22267	3·68220	0·22433
9·5	3·028879	2·13647	5·15199	0·40661	**9·5**	2·234727	3·25108	3·83550	0·22134
10·0	3·166904	2·15766	5·40045	0·40117	**10·0**	2·337141	3·27873	3·99209	0·21849

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

$3d\sigma_g$

R	p	σ	$-A'$	$-E$
0·0	0·000000	2·00000	6·00000	0·44444
0·2	(0·066684)	(1·99924)	6·00212	(0·44467)
0·4	(0·133470)	(1·99693)	6·00848	(0·44536)
0·6	0·200465	1·99304	6·01915	0·44651
0·8	0·267782	1·98750	6·03420	0·44817
1·0	0·335548	1·98020	6·05374	0·45037
1·2	0·403902	1·97102	6·07795	0·45316
1·4	0·473004	1·95981	6·10705	0·45660
1·6	0·543034	1·94641	6·14132	0·46076
1·8	0·614193	1·93068	6·18111	0·46572
2·0	0·686698	1·91249	6·22686	0·47155
2·2	0·760776	1·89178	6·27910	0·47833
2·4	0·836645	1·86860	6·33845	0·48609
2·6	0·914485	1·84313	6·40560	0·49484
2·8	0·994411	1·81574	6·48125	0·50452
3·0	1·076455	1·78693	6·56613	0·51500
3·2	1·16055	1·75732	6·66089	0·52612
3·4	1·24648	1·72769	6·76604	0·53761
3·6	1·33393	1·69879	6·88196	0·54919
3·8	1·42254	1·67128	7·00882	0·56056
4·0	1·51188	1·64571	7·14665	0·57145
4·2	1·60153	1·62249	7·29530	0·58161
4·4	1·69108	1·60189	7·45449	0·59086
4·6	1·78016	1·58404	7·62389	0·59905
4·8	1·86847	1·56894	7·80307	0·60611
5·0	1·95579	1·55651	7·99160	0·61202
5·5	2·16842	1·53641	8·50054	0·62176
6·0	2·37169	1·52985	9·05721	0·62499
6·5	2·56508	1·53404	9·65443	0·62292
7·0	2·74887	1·54650	10·28578	0·61684
7·5	2·92379	1·56517	10·94565	0·60790
8·0	3·09069	1·58842	11·62919	0·59702
8·5	3·25049	1·61499	12·33247	0·58495
9·0	3·40404	1·64391	13·05223	0·57222
9·5	3·55212	1·67446	13·78568	0·55923
10·0	3·69538	1·70608	14·53058	0·54623

$4f\sigma_u$

R	p	σ	$-A'$	$-E$
0·0	0·000000	3·00000	12·00000	0·25000
0·2	(0·050003)	(2·99975)	12·00122	(0·25003)
0·4	(0·100025)	(2·99898)	12·00489	(0·25013)
0·6	0·150086	2·99771	12·01101	0·25029
0·8	0·200204	2·99592	12·01960	0·25051
1·0	0·250400	2·99361	12·03067	0·25080
1·2	0·300693	2·99078	12·04423	0·25116
1·4	0·351105	2·98741	12·06032	0·25158
1·6	0·401658	2·98349	12·07896	0·25208
1·8	0·452374	2·97901	12·10019	0·25265
2·0	0·503277	2·97395	12·12404	0·25329
2·2	0·554393	2·96830	12·15057	0·25401
2·4	0·605749	2·96204	12·17983	0·25481
2·6	0·657374	2·95513	12·21188	0·25570
2·8	0·709301	2·94755	12·24679	0·25669
3·0	0·761563	2·93927	12·28464	0·25777
3·2	0·814199	2·93025	12·32552	0·25895
3·4	0·867250	2·92044	12·36954	0·26025
3·6	0·920763	2·90980	12·41681	0·26167
3·8	0·974787	2·89829	12·46747	0·26322
4·0	1·029378	2·88584	12·52166	0·26491
4·2	1·084596	2·87241	12·57955	0·26675
4·4	1·140504	2·85794	12·64135	0·26875
4·6	1·197174	2·84238	12·70727	0·27093
4·8	1·254679	2·82568	12·77753	0·27330
5·0	1·313091	2·80781	12·85241	0·27587
5·5	1·46355	2·75798	13·06167	0·28324
6·0	1·62109	2·70121	13·30632	0·29199
6·5	1·78611	2·63919	13·59100	0·30203
7·0	1·95812	2·57486	13·91909	0·31300
7·5	2·13569	2·51174	14·29184	0·32435
8·0	2·31684	2·45297	14·70816	0·33549
8·5	2·49948	2·40071	15·16517	0·34588
9·0	2·68179	2·35597	15·65903	0·35516
9·5	2·86244	2·31885	16·18559	0·36315
10·0	3·04045	2·28899	16·74077	0·36977

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

TABLE 1. THE BASIC PARAMETERS (*cont.*)

	$2p\,\pi_u$				$3d\,\pi_g$				
R	p	σ	$-A'$	$-E$	R	p	σ	$-A'$	$-E$
0·0	0·00000	0·00000	2·00000	1·00000	**0·0**	0·000000	1·00000	6·00000	0·44444
0·2	0·09987	(0·00260)	2·00798	(0·99740)	**0·2**	(0·066676)	(0·99956)	6·00254	(0·44457)
0·4	0·19899	(0·01015)	2·03167	(0·98993)	**0·4**	(0·133402)	(0·99846)	6·01016	(0·44490)
0·6	0·29677	(0·02176)	2·07042	(0·97860)	**0·6**	(0·200224)	(0·99665)	6·02290	(0·44544)
0·8	0·39281	0·03659	2·12333	0·96439	**0·8**	0·267188	0·99415	6·04078	0·44618
1·0	0·48688	0·05389	2·18938	0·94821	**1·0**	0·334332	0·99104	6·06383	0·44711
1·2	0·57886	0·07303	2·26755	0·93078	**1·2**	0·401683	0·98743	6·09210	0·44819
1·4	0·66873	0·09352	2·35684	0·91265	**1·4**	0·469258	0·98343	6·12564	0·44939
1·6	0·75650	0·11499	2·45633	0·89422	**1·6**	0·537065	0·97915	6·16450	0·45069
1·8	0·84225	0·13713	2·56517	0·87579	**1·8**	0·605100	0·97471	6·20871	0·45203
2·0	0·92604	0·15973	2·68260	0·85755	**2·0**	0·673350	0·97022	6·25829	0·45340
2·2	1·00795	0·18264	2·80794	0·83965	**2·2**	0·741788	0·96581	6·31325	0·45475
2·4	1·08809	0·20570	2·94054	0·82218	**2·4**	0·810376	0·96159	6·37358	0·45605
2·6	1·16653	0·22882	3·07987	0·80521	**2·6**	0·879082	0·95763	6·43926	0·45727
2·8	1·24338	0·25192	3·22541	0·78878	**2·8**	0·947858	0·95403	6·51024	0·45839
3·0	1·31871	0·27495	3·37672	0·77289	**3·0**	1·016655	0·95085	6·58645	0·45937
3·2	1·39261	0·29785	3·53337	0·75756	**3·2**	1·085421	0·94816	6·66780	0·46021
3·4	1·46514	0·32060	3·69499	0·74278	**3·4**	1·154112	0·94599	6·75420	0·46089
3·6	1·53639	0·34316	3·86125	0·72854	**3·6**	1·222679	0·94435	6·84553	0·46140
3·8	1·60642	0·36551	4·03183	0·71484	**3·8**	1·291080	0·94327	6·94165	0·46174
4·0	1·67529	0·38764	4·20645	0·70165	**4·0**	1·359273	0·94275	7·04244	0·46191
4·2	1·74307	0·40954	4·38486	0·68896	**4·2**	1·427223	0·94278	7·14774	0·46190
4·4	1·80981	0·43119	4·56679	0·67674	**4·4**	1·494895	0·94335	7·25743	0·46172
4·6	1·87557	0·45259	4·75203	0·66498	**4·6**	1·562264	0·94444	7·37133	0·46137
4·8	1·94039	0·47373	4·94038	0·65366	**4·8**	1·629304	0·94604	7·48930	0·46087
5·0	2·00432	0·49461	5·13164	0·64277	**5·0**	1·696000	0·94811	7·61121	0·46023
5·5	2·16054	0·54566	5·62144	0·61725	**5·5**	1·861112	0·95522	7·93213	0·45801
6·0	2·31211	0·59503	6·12587	0·59398	**6·0**	2·023781	0·96475	8·27437	0·45508
6·5	2·45955	0·64275	6·64279	0·57272	**6·5**	2·183942	0·97627	8·63580	0·45156
7·0	2·60336	0·68883	7·17030	0·55326	**7·0**	2·341593	0·98942	9·01448	0·44760
7·5	2·74395	0·73328	7·70674	0·53542	**7·5**	2·496790	1·00386	9·40862	0·44330
8·0	2·88172	0·77612	8·25062	0·51902	**8·0**	2·649626	1·01929	9·81663	0·43878
8·5	3·01702	0·81735	8·80057	0·50394	**8·5**	2·800213	1·03548	10·23705	0·43411
9·0	3·15017	0·85699	9·35535	0·49005	**9·0**	2·948671	1·05222	10·66857	0·42937
9·5	3·28145	0·89507	9·91378	0·47725	**9·5**	3·095131	1·06934	11·11000	0·42459
10·0	3·41113	0·93158	10·47479	0·46543	**10·0**	3·239724	1·08668	11·56029	0·41983

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

TABLE 2. THE COEFFICIENTS OF THE μ EXPANSION ((7) OF TEXT)

$1s\sigma_g$

R	f_0	f_2	f_4	f_6	f_8	f_{10}	f_{12}	f_{14}
0·0	1·0000	0·00000	0·000000	—	—	—	—	—
0·2	1·0020	0·00430	0·000003	—	—	—	—	—
0·4	1·0081	0·01621	0·000040	—	—	—	—	—
0·6	1·0171	0·03432	0·000177	0·000000	—	—	—	—
0·8	1·0287	0·05774	0·000495	0·000002	—	—	—	—
1·0	1·0426	0·08598	0·001076	0·000006	—	—	—	—
1·2	1·0587	0·11886	0·002014	0·000014	—	—	—	—
1·4	1·0769	0·15634	0·003407	0·000031	—	—	—	—
1·6	1·0973	0·19859	0·005362	0·000061	0·000000	—	—	—
1·8	1·1199	0·24584	0·008001	0·000109	0·000001	—	—	—
2·0	1·1450	0·29844	0·011461	0·000184	0·000002	—	—	—
2·2	1·1725	0·35680	0·015898	0·000295	0·000003	—	—	—
2·4	1·2028	0·42144	0·021492	0·000456	0·000005	—	—	—
2·6	1·2360	0·49296	0·028449	0·000683	0·000009	—	—	—
2·8	1·2724	0·57208	0·037006	0·000995	0·000015	—	—	—
3·0	1·3124	0·65953	0·047438	0·001418	0·000023	—	—	—
3·2	1·3562	0·7563	0·060064	0·001981	0·000036	0·000000	—	—
3·4	1·4043	0·8632	0·07525	0·002723	0·000054	0·000001	—	—
3·6	1·4569	0·9816	0·09342	0·003690	0·000080	0·000001	—	—
3·8	1·5146	1·1126	0·11506	0·004937	0·000117	0·000002	—	—
4·0	1·5780	1·2575	0·14072	0·006535	0·000167	0·000003	—	—
4·2	1·6475	1·4179	0·17106	0·008565	0·000236	0·000004	—	—
4·4	1·7236	1·5956	0·20680	0·011129	0·000330	0·000006	—	—
4·6	1·8071	1·7922	0·24877	0·014348	0·000456	0·000009	—	—
4·8	1·8988	2·0099	0·29792	0·018365	0·000624	0·000013	—	—
5·0	1·9992	2·2507	0·35531	0·023352	0·000846	0·000019	0·000000	—
5·5	2·2942	2·9709	0·5432	0·04151	0·001751	0·000047	0·000001	—
6·0	2·6640	3·8956	0·8141	0·07144	0·003469	0·000107	0·000002	—
6·5	3·1259	5·0798	1·1990	0·11960	0·006620	0·000233	0·000006	—
7·0	3·7012	6·5911	1·7388	0·19533	0·01221	0·000487	0·000013	0·000000
7·5	4·4164	8·515	2·4873	0·31201	0·02187	0·000980	0·000030	0·000001
8·0	5·3036	10·957	3·5141	0·48848	0·03811	0·001904	0·000066	0·000002
8·5	6·4029	14·053	4·9103	0·75111	0·06478	0·003587	0·000138	0·000004
9·0	7·7649	17·971	6·7945	1·13645	0·10772	0·006572	0·000280	0·000009

$2s\sigma_g$

R	f_0	f_2	f_4	f_6	f_8	f_{10}	f_{12}
0·0	1·0000	0·00000	—	—	—	—	—
0·2	1·0006	0·00109	0·000000	—	—	—	—
0·4	1·0020	0·00423	0·000003	—	—	—	—
0·6	1·0045	0·00919	0·000013	—	—	—	—
0·8	1·0079	0·01580	0·000038	—	—	—	—
1·0	1·0120	0·02393	0·000087	—	—	—	—
1·2	1·0167	0·03352	0·000169	0·000000	—	—	—
1·4	1·0221	0·04448	0·000296	0·000001	—	—	—
1·6	1·0282	0·05680	0·000479	0·000002	—	—	—
1·8	1·0349	0·07046	0·000730	0·000003	—	—	—
2·0	1·0423	0·08546	0·001064	0·000006	—	—	—
2·2	1·0503	0·10180	0·001494	0·000009	—	—	—
2·4	1·0590	0·11950	0·002035	0·000014	—	—	—
2·6	1·0683	0·13859	0·002706	0·000022	—	—	—
2·8	1·0782	0·15911	0·003523	0·000033	—	—	—
3·0	1·0889	0·18110	0·004505	0·000047	—	—	—
3·2	1·1002	0·20463	0·005674	0·000066	0·000000	—	—
3·4	1·1122	0·22974	0·007050	0·000090	0·000001	—	—
3·6	1·1250	0·25651	0·008660	0·000122	0·000001	—	—
3·8	1·1386	0·28500	0·010527	0·000162	0·000001	—	—
4·0	1·1529	0·31530	0·012680	0·000213	0·000002	—	—
4·2	1·1681	0·34749	0·015150	0·000275	0·000003	—	—
4·4	1·1842	0·38167	0·017970	0·000353	0·000004	—	—
4·6	1·2012	0·41794	0·021173	0·000447	0·000005	—	—
4·8	1·2191	0·45642	0·024798	0·000561	0·000007	—	—
5·0	1·2380	0·49722	0·028887	0·000698	0·000009	—	—
5·5	1·2899	0·61022	0·04144	0·001169	0·000018	—	—
6·0	1·3492	0·74070	0·05796	0·001883	0·000034	0·000000	—
6·5	1·4167	0·8912	0·07942	0·002937	0·000060	0·000001	—
7·0	1·4935	1·0647	0·10697	0·004459	0·000102	0·000001	—
7·5	1·5809	1·2643	0·14197	0·006615	0·000170	0·000003	—
8·0	1·6801	1·4938	0·18606	0·009620	0·000274	0·000005	—
8·5	1·7924	1·7573	0·24114	0·013747	0·000432	0·000009	—
9·0	1·9195	2·0593	0·30945	0·019342	0·000666	0·000015	—
9·5	2·0630	2·4050	0·39360	0·026839	0·001009	0·000024	0·000000
10·0	2·2248	2·8000	0·49661	0·036771	0·001503	0·000039	0·000001

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

TABLE 2. THE COEFFICIENTS OF THE μ EXPANSION ((7) OF TEXT) (*cont.*)

$3s\sigma_g$

R	f_0	f_2	f_4	f_6	f_8	f_{10}
0·0	1·0000	0·00000	—	—	—	—
0·2	1·0002	0·00049	0·000000	—	—	—
0·4	1·0009	0·00191	0·000001	—	—	—
0·6	1·0021	0·00419	0·000003	—	—	—
0·8	1·0036	0·00728	0·000008	—	—	—
1·0	1·0055	0·01112	0·000019	—	—	—
1·2	1·0078	0·01568	0·000038	—	—	—
1·4	1·0105	0·02094	0·000067	—	—	—
1·6	1·0134	0·02688	0·000109	—	—	—
1·8	1·0167	0·03348	0·000169	0·000000	—	—
2·0	1·0202	0·04073	0·000249	0·000001	—	—
2·2	1·0241	0·04863	0·000353	0·000001	—	—
2·4	1·0284	0·05718	0·000485	0·000002	—	—
2·6	1·0329	0·06637	0·000650	0·000003	—	—
2·8	1·0378	0·07621	0·000851	0·000004	—	—
3·0	1·0429	0·08671	0·001094	0·000006	—	—
3·2	1·0484	0·09787	0·001384	0·000008	—	—
3·4	1·0542	0·10971	0·001726	0·000011	—	—
3·6	1·0603	0·12222	0·002126	0·000015	—	—
3·8	1·0667	0·13544	0·002589	0·000021	—	—
4·0	1·0735	0·14937	0·003123	0·000027	—	—
4·2	1·0806	0·16403	0·003733	0·000036	—	—
4·4	1·0881	0·17944	0·004427	0·000046	—	—
4·6	1·0959	0·19563	0·005212	0·000058	—	—
4·8	1·1040	0·21261	0·006097	0·000073	0·000000	—
5·0	1·1126	0·23041	0·007089	0·000091	0·000001	—
5·5	1·1356	0·27867	0·010099	0·000153	0·000001	—
6·0	1·1611	0·33267	0·013990	0·000245	0·000002	—
6·5	1·1894	0·39291	0·018939	0·000380	0·000004	—
7·0	1·2207	0·46000	0·025147	0·000572	0·000007	—
7·5	1·2552	0·53461	0·032845	0·000839	0·000012	—
8·0	1·2932	0·61747	0·042299	0·001204	0·000019	—
8·5	1·3351	0·70941	0·053813	0·001696	0·000029	0·000000
9·0	1·3810	0·81133	0·067729	0·002347	0·000045	0·000001
9·5	1·4314	0·9242	0·08444	0·003202	0·000067	0·000001
10·0	1·4867	1·0492	0·10439	0·004310	0·000098	0·000001

$2p\sigma_u$

R	f_1	f_3	f_5	f_7	f_9	f_{11}	f_{13}
0·0	1·0000	0·000000	—	—	—	—	—
0·2	1·0006	0·000402	0·000000	—	—	—	—
0·4	1·0025	0·001638	0·000001	—	—	—	—
0·6	1·0057	0·003794	0·000004	—	—	—	—
0·8	1·0105	0·007009	0·000014	—	—	—	—
1·0	1·0171	0·01146	0·000037	—	—	—	—
1·2	1·0258	0·01732	0·000083	0·000000	—	—	—
1·4	1·0368	0·02474	0·000168	0·000001	—	—	—
1·6	1·0502	0·03381	0·000310	0·000001	—	—	—
1·8	1·0660	0·04461	0·000532	0·000003	—	—	—
2·0	1·0842	0·05717	0·000861	0·000006	—	—	—
2·2	1·1048	0·07155	0·001326	0·000012	—	—	—
2·4	1·1280	0·08778	0·001959	0·000021	—	—	—
2·6	1·1537	0·10594	0·002796	0·000035	—	—	—
2·8	1·1820	0·12608	0·003876	0·000057	0·000000	—	—
3·0	1·2129	0·14832	0·005241	0·000089	0·000001	—	—
3·2	1·2464	0·17276	0·006940	0·000135	0·000002	—	—
3·4	1·2828	0·19952	0·009023	0·000197	0·000003	—	—
3·6	1·3222	0·22877	0·011547	0·000282	0·000004	—	—
3·8	1·3646	0·26067	0·014578	0·000395	0·000006	—	—
4·0	1·4102	0·29540	0·018184	0·000543	0·000010	—	—
4·2	1·4593	0·33318	0·022443	0·000734	0·000014	—	—
4·4	1·5120	0·37423	0·027442	0·000979	0·000021	—	—
4·6	1·5686	0·41882	0·033275	0·001288	0·000030	0·000000	—
4·8	1·6293	0·46722	0·040049	0·001675	0·000042	0·000001	—
5·0	1·6944	0·51974	0·047882	0·002156	0·000058	0·000001	—
5·5	1·8784	0·6714	0·072989	0·003896	0·000124	0·000003	—
6·0	2·0973	0·8572	0·10804	0·006717	0·000250	0·000006	—
6·5	2·3577	1·0849	0·15620	0·011155	0·000477	0·000014	0·000000
7·0	2·6676	1·3639	0·22158	0·017963	0·000875	0·000028	0·000001
7·5	3·0369	1·7061	0·30950	0·028193	0·001548	0·000057	0·000001
8·0	3·4774	2·1260	0·42668	0·043288	0·002655	0·000109	0·000003
8·5	4·0036	2·6415	0·58183	0·065247	0·004438	0·000203	0·000007
9·0	4·6331	3·2748	0·78609	0·09683	0·007255	0·000366	0·000013

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

$3p\,\sigma_u$

R	f_1	f_3	f_5	f_7	f_9	f_{11}
0·0	1·0000	0·00000	—	—	—	—
0·2	1·0003	0·00018	—	—	—	—
0·4	1·0011	0·00072	0·000000	—	—	—
0·6	1·0025	0·00165	0·000001	—	—	—
0·8	1·0045	0·00301	0·000003	—	—	—
1·0	1·0072	0·00482	0·000007	—	—	—
1·2	1·0107	0·00710	0·000014	—	—	—
1·4	1·0148	0·00987	0·000027	—	—	—
1·6	1·0196	0·01311	0·000048	—	—	—
1·8	1·0251	0·01682	0·000078	—	—	—
2·0	1·0312	0·02097	0·000121	0·000000	—	—
2·2	1·0380	0·02557	0·000179	0·000001	—	—
2·4	1·0454	0·03060	0·000255	0·000001	—	—
2·6	1·0535	0·03607	0·000352	0·000002	—	—
2·8	1·0621	0·04197	0·000473	0·000003	—	—
3·0	1·0713	0·04830	0·000621	0·000004	—	—
3·2	1·0811	0·05508	0·000801	0·000006	—	—
3·4	1·0915	0·06229	0·001016	0·000008	—	—
3·6	1·1025	0·06996	0·001270	0·000011	—	—
3·8	1·1142	0·07809	0·001568	0·000015	—	—
4·0	1·1265	0·08670	0·001913	0·000020	—	—
4·2	1·1394	0·09577	0·002311	0·000027	—	—
4·4	1·1529	0·10537	0·002768	0·000035	—	—
4·6	1·1672	0·11546	0·003287	0·000045	—	—
4·8	1·1820	0·12607	0·003870	0·000057	0·000000	—
5·0	1·1975	0·13723	0·004538	0·000072	0·000001	—
5·5	1·2394	0·16759	0·006564	0·000124	0·000001	—
6·0	1·2858	0·20175	0·009206	0·000203	0·000003	—
6·5	1·3372	0·24005	0·012587	0·000320	0·000005	—
7·0	1·3938	0·28289	0·016850	0·000487	0·000008	—
7·5	1·4561	0·33074	0·022158	0·000721	0·000014	—
8·0	1·5246	0·38409	0·028697	0·001043	0·000023	0·000000
8·5	1·5997	0·44354	0·036679	0·001479	0·000035	0·000001
9·0	1·6820	0·50971	0·046349	0·002059	0·000054	0·000001
9·5	1·7723	0·58333	0·057984	0·002822	0·000082	0·000002
10·0	1·8710	0·66522	0·071902	0·003815	0·000121	0·000003

$4p\,\sigma_u$

R	f_1	f_3	f_5	f_7	f_9
0·0	1·0000	0·000000	—	—	—
0·2	1·0001	0·000100	—	—	—
0·4	1·0006	0·000404	—	—	—
0·6	1·0014	0·000922	0·000000	—	—
0·8	1·0025	0·001665	0·000001	—	—
1·0	1·0040	0·002647	0·000002	—	—
1·2	1·0058	0·003873	0·000004	—	—
1·4	1·0080	0·005341	0·000008	—	—
1·6	1·0105	0·007046	0·000014	—	—
1·8	1·0134	0·008982	0·000023	—	—
2·0	1·0166	0·011140	0·000035	—	—
2·2	1·0202	0·013517	0·000051	—	—
2·4	1·0240	0·016107	0·000072	—	—
2·6	1·0282	0·018909	0·000099	—	—
2·8	1·0326	0·021919	0·000132	0·000000	—
3·0	1·0374	0·025136	0·000173	0·000001	—
3·2	1·0424	0·028561	0·000223	0·000001	—
3·4	1·0478	0·032192	0·000282	0·000001	—
3·6	1·0534	0·036030	0·000351	0·000002	—
3·8	1·0593	0·040076	0·000432	0·000002	—
4·0	1·0656	0·044332	0·000526	0·000003	—
4·2	1·0720	0·048798	0·000634	0·000004	—
4·4	1·0788	0·053479	0·000757	0·000005	—
4·6	1·0859	0·058374	0·000896	0·000007	—
4·8	1·0932	0·063488	0·001054	0·000008	—
5·0	1·1009	0·068823	0·001231	0·000011	—
5·5	1·1214	0·08315	0·001767	0·000018	—
6·0	1·1439	0·09894	0·002458	0·000029	—
6·5	1·1683	0·11627	0·003330	0·000046	0·000000
7·0	1·1947	0·13520	0·004414	0·000069	0·000001
7·5	1·2232	0·15583	0·005742	0·000102	0·000001
8·0	1·2540	0·17827	0·007350	0·000146	0·000002
8·5	1·2870	0·20262	0·009278	0·000205	0·000003
9·0	1·3225	0·22902	0·011570	0·000283	0·000004
9·5	1·3605	0·25759	0·014273	0·000383	0·000006
10·0	1·4012	0·28848	0·017441	0·000511	0·000009

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

TABLE 2. THE COEFFICIENTS OF THE μ EXPANSION ((7) OF TEXT) (*cont.*)

	$3d\sigma_g$						
R	f_0	f_2	f_4	f_6	f_8	f_{10}	f_{12}
0·0	−0·000000	1·00000	0·000000	—	—	—	—
0·2	−0·000099	0·99988	0·000109	—	—	—	—
0·4	−0·000396	0·99953	0·000436	—	—	—	—
0·6	−0·000893	0·99896	0·000983	0·000000	—	—	—
0·8	−0·001594	0·99813	0·001753	0·000001	—	—	—
1·0	−0·002504	0·99706	0·002749	0·000003	—	—	—
1·2	−0·003628	0·99573	0·003977	0·000005	—	—	—
1·4	−0·004978	0·99413	0·005446	0·000010	—	—	—
1·6	−0·006563	0·99224	0·007164	0·000018	—	—	—
1·8	−0·008398	0·99004	0·009143	0·000029	—	—	—
2·0	−0·010502	0·98751	0·011400	0·000045	—	—	—
2·2	−0·012894	0·98463	0·013951	0·000068	—	—	—
2·4	−0·015598	0·98135	0·016815	0·000099	0·000000	—	—
2·6	−0·018641	0·97764	0·020014	0·000141	0·000001	—	—
2·8	−0·022046	0·97347	0·023566	0·000196	0·000001	—	—
3·0	−0·025835	0·96878	0·027485	0·000268	0·000001	—	—
3·2	−0·030026	0·96356	0·031782	0·000360	0·000002	—	—
3·4	−0·034627	0·95780	0·036454	0·000477	0·000003	—	—
3·6	−0·039633	0·95147	0·041490	0·000621	0·000005	—	—
3·8	−0·045031	0·94460	0·046871	0·000799	0·000007	—	—
4·0	−0·050799	0·93720	0·052567	0·001012	0·000010	—	—
4·2	−0·056902	0·92932	0·058546	0·001265	0·000014	—	—
4·4	−0·063298	0·92101	0·064769	0·001561	0·000019	—	—
4·6	−0·069946	0·91234	0·071198	0·001902	0·000026	—	—
4·8	−0·076796	0·90335	0·077799	0·002291	0·000035	—	—
5·0	−0·083803	0·89412	0·084541	0·002730	0·000046	0·000000	—
5·5	−0·10171	0·87047	0·10183	0·004051	0·000083	0·000001	—
6·0	−0·11967	0·84683	0·11954	0·005706	0·000140	0·000002	—
6·5	−0·13722	0·82401	0·13753	0·007709	0·000222	0·000004	—
7·0	−0·15408	0·80262	0·15587	0·010078	0·000334	0·000007	—
7·5	−0·17011	0·78300	0·17464	0·012840	0·000483	0·000011	—
8·0	−0·18526	0·76529	0·19400	0·016032	0·000676	0·000017	0·000000
8·5	−0·19964	0·74950	0·21416	0·019698	0·000921	0·000026	0·000001
9·0	−0·21332	0·73555	0·23529	0·023896	0·001230	0·000039	0·000001
9·5	−0·22642	0·72328	0·25760	0·028692	0·001614	0·000055	0·000001
10·0	−0·23907	0·71257	0·28128	0·034162	0·002088	0·000078	0·000002

	$4f\sigma_u$					
R	f_1	f_3	f_5	f_7	f_9	f_{11}
0·0	−0·000000	1·00000	0·000000	—	—	—
0·2	−0·000043	1·00003	0·000044	—	—	—
0·4	−0·000172	1·00011	0·000176	—	—	—
0·6	−0·000386	1·00024	0·000397	—	—	—
0·8	−0·000687	1·00043	0·000707	—	—	—
1·0	−0·001075	1·00067	0·001107	0·000000	—	—
1·2	−0·001550	1·00096	0·001596	0·000001	—	—
1·4	−0·002114	1·00131	0·002177	0·000002	—	—
1·6	−0·002766	1·00172	0·002850	0·000003	—	—
1·8	−0·003509	1·00218	0·003617	0·000005	—	—
2·0	−0·004344	1·00270	0·004479	0·000008	—	—
2·2	−0·005272	1·00327	0·005438	0·000011	—	—
2·4	−0·006294	1·00390	0·006496	0·000016	—	—
2·6	−0·007413	1·00460	0·007656	0·000022	—	—
2·8	−0·008631	1·00535	0·008920	0·000030	—	—
3·0	−0·009952	1·00617	0·010291	0·000040	—	—
3·2	−0·011376	1·00706	0·011773	0·000052	—	—
3·4	−0·012908	1·00801	0·013370	0·000067	—	—
3·6	−0·014551	1·00903	0·015086	0·000085	—	—
3·8	−0·016311	1·01013	0·016927	0·000107	0·000000	—
4·0	−0·018192	1·01130	0·018898	0·000134	0·000001	—
4·2	−0·020199	1·01255	0·021005	0·000165	0·000001	—
4·4	−0·022338	1·01389	0·023258	0·000202	0·000001	—
4·6	−0·024616	1·01532	0·025664	0·000246	0·000001	—
4·8	−0·027041	1·01684	0·028232	0·000297	0·000002	—
5·0	−0·029621	1·01846	0·030974	0·000356	0·000002	—
5·5	−0·036810	1·02298	0·038659	0·000553	0·000004	—
6·0	−0·045172	1·02830	0·047696	0·000837	0·000008	—
6·5	−0·054849	1·03451	0·058284	0·001242	0·000014	—
7·0	−0·065930	1·04170	0·070599	0·001808	0·000025	—
7·5	−0·078432	1·04995	0·084749	0·002583	0·000043	0·000000
8·0	−0·092296	1·05928	0·10078	0·003616	0·000070	0·000001
8·5	−0·10741	1·06971	0·11869	0·004959	0·000112	0·000002
9·0	−0·12363	1·08119	0·13844	0·006664	0·000174	0·000003
9·5	−0·14084	1·09373	0·16002	0·008784	0·000261	0·000005
10·0	−0·15891	1·10735	0·18341	0·01137	0·000381	0·000008

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

$2p\,\pi_u$

R	f_0	f_2	f_4	f_6	f_8	f_{10}
0·0	1·0000	0·000000	—	—	—	—
0·2	1·0002	0·000133	—	—	—	—
0·4	1·0008	0·000529	0·000000	—	—	—
0·6	1·0018	0·001179	0·000001	—	—	—
0·8	1·0031	0·002073	0·000002	—	—	—
1·0	1·0048	0·003196	0·000005	—	—	—
1·2	1·0068	0·004539	0·000010	—	—	—
1·4	1·0091	0·006089	0·000019	—	—	—
1·6	1·0117	0·007839	0·000031	—	—	—
1·8	1·0146	0·009780	0·000047	—	—	—
2·0	1·0177	0·011907	0·000070	—	—	—
2·2	1·0211	0·014214	0·000099	0·000000	—	—
2·4	1·0248	0·016698	0·000136	0·000001	—	—
2·6	1·0287	0·019358	0·000182	0·000001	—	—
2·8	1·0329	0·022191	0·000237	0·000001	—	—
3·0	1·0372	0·025198	0·000303	0·000002	—	—
3·2	1·0418	0·028379	0·000382	0·000003	—	—
3·4	1·0467	0·031736	0·000474	0·000004	—	—
3·6	1·0518	0·035270	0·000580	0·000005	—	—
3·8	1·0572	0·038985	0·000702	0·000007	—	—
4·0	1·0628	0·042885	0·000842	0·000009	—	—
4·2	1·0686	0·046973	0·001001	0·000012	—	—
4·4	1·0747	0·051254	0·001180	0·000015	—	—
4·6	1·0811	0·055734	0·001381	0·000019	—	—
4·8	1·0877	0·060419	0·001606	0·000024	—	—
5·0	1·0946	0·065316	0·001858	0·000030	0·000000	—
5·5	1·1130	0·07853	0·002611	0·000048	0·000001	—
6·0	1·1333	0·09325	0·003572	0·000076	0·000001	—
6·5	1·1557	0·10963	0·004781	0·000116	0·000002	—
7·0	1·1803	0·12784	0·006287	0·000171	0·000003	—
7·5	1·2074	0·14812	0·008143	0·000247	0·000005	—
8·0	1·2373	0·17072	0·010415	0·000350	0·000007	—
8·5	1·2702	0·19592	0·013181	0·000486	0·000011	—
9·0	1·3065	0·22406	0·016531	0·000667	0·000017	—
9·5	1·3466	0·25552	0·020575	0·000903	0·000025	0·000000
10·0	1·3910	0·29074	0·025436	0·001210	0·000036	0·000001

$3d\,\pi_g$

R	f_1	f_3	f_5	f_7	f_9
0·0	1·0000	0·000000	—	—	—
0·2	1·0001	0·000054	—	—	—
0·4	1·0005	0·000217	—	—	—
0·6	1·0012	0·000491	—	—	—
0·8	1·0022	0·000876	0·000000	—	—
1·0	1·0034	0·001373	0·000001	—	—
1·2	1·0049	0·001987	0·000002	—	—
1·4	1·0068	0·002717	0·000003	—	—
1·6	1·0089	0·003567	0·000006	—	—
1·8	1·0113	0·004540	0·000009	—	—
2·0	1·0140	0·005639	0·000014	—	—
2·2	1·0171	0·006866	0·000021	—	—
2·4	1·0204	0·008225	0·000030	—	—
2·6	1·0241	0·009717	0·000042	—	—
2·8	1·0281	0·011347	0·000057	—	—
3·0	1·0325	0·013115	0·000076	—	—
3·2	1·0372	0·015024	0·000099	0·000000	—
3·4	1·0422	0·017077	0·000128	0·000001	—
3·6	1·0475	0·019275	0·000162	0·000001	—
3·8	1·0532	0·021620	0·000203	0·000001	—
4·0	1·0592	0·024115	0·000251	0·000002	—
4·2	1·0656	0·026762	0·000307	0·000002	—
4·4	1·0723	0·029563	0·000372	0·000003	—
4·6	1·0794	0·032521	0·000447	0·000004	—
4·8	1·0868	0·035637	0·000533	0·000005	—
5·0	1·0946	0·038915	0·000631	0·000006	—
5·5	1·1156	0·04783	0·000934	0·000011	—
6·0	1·1389	0·05784	0·001337	0·000018	—
6·5	1·1645	0·06897	0·001858	0·000029	0·000000
7·0	1·1925	0·08132	0·002520	0·000045	0·000001
7·5	1·2232	0·09496	0·003347	0·000068	0·000001
8·0	1·2565	0·10999	0·004368	0·000101	0·000002
8·5	1·2927	0·12651	0·005614	0·000144	0·000002
9·0	1·3318	0·14465	0·007120	0·000203	0·000004
9·5	1·3741	0·16455	0·008925	0·000280	0·000006
10·0	1·4199	0·18636	0·011074	0·000381	0·000009

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

TABLE 3. THE COEFFICIENTS OF THE λ EXPANSION ((13) OF TEXT)

	$1s\sigma_g$			$2s\sigma_g$					
R	g_0	g_1	g_2	R	g_0	g_1	g_2	g_3	g_4
0·0	1	0·0000	0·0000	**0·0**	1	−1·0000	0·0000	0·0000	0·0000
0·2	1	0·0002	0·0000	**0·2**	1	−1·2136	−0·0002	−0·0000	−0·0000
0·4	1	0·0010	0·0001	**0·4**	1	−1·4392	−0·0014	−0·0001	−0·0000
0·6	1	0·0024	0·0002	**0·6**	1	−1·6663	−0·0042	−0·0004	−0·0001
0·8	1	0·0042	0·0002	**0·8**	1	−1·8919	−0·0087	−0·0006	−0·0001
1·0	1	0·0062	0·0003	**1·0**	1	−2·1146	−0·0148	−0·0008	−0·0001
1·2	1	0·0083	0·0004	**1·2**	1	−2·3342	−0·0225	−0·0011	−0·0001
1·4	1	0·0105	0·0004	**1·4**	1	−2·5506	−0·0317	−0·0013	−0·0002
1·6	1	0·0126	0·0004	**1·6**	1	−2·7639	−0·0423	−0·0015	−0·0002
1·8	1	0·0147	0·0004	**1·8**	1	−2·9743	−0·0541	−0·0017	−0·0002
2·0	1	0·0168	0·0004	**2·0**	1	−3·1818	−0·0670	−0·0018	−0·0002
2·2	1	0·0187	0·0003	**2·2**	1	−3·3868	−0·0811	−0·0019	−0·0002
2·4	1	0·0206	0·0003	**2·4**	1	−3·5893	−0·0961	−0·0020	−0·0001
2·6	1	0·0223	0·0003	**2·6**	1	−3·7895	−0·1121	−0·0020	−0·0001
2·8	1	0·0239	0·0003	**2·8**	1	−3·9876	−0·1289	−0·0020	−0·0001
3·0	1	0·0255	0·0003	**3·0**	1	−4·1837	−0·1466	−0·0020	−0·0001
3·2	1	0·0269	0·0003	**3·2**	1	−4·3780	−0·1649	−0·0019	−0·0001
3·4	1	0·0281	0·0002	**3·4**	1	−4·5706	−0·1840	−0·0019	−0·0001
3·6	1	0·0293	0·0002	**3·6**	1	−4·7617	−0·2036	−0·0018	−0·0001
3·8	1	0·0304	0·0002	**3·8**	1	−4·9514	−0·2238	−0·0018	−0·0001
4·0	1	0·0313	0·0002	**4·0**	1	−5·1398	−0·2445	−0·0017	−0·0001
4·2	1	0·0321	0·0002	**4·2**	1	−5·3270	−0·2656	−0·0016	−0·0001
4·4	1	0·0328	0·0002	**4·4**	1	−5·5132	−0·2871	−0·0014	−0·0001
4·6	1	0·0334	0·0001	**4·6**	1	−5·6983	−0·3091	−0·0013	—
4·8	1	0·0339	0·0001	**4·8**	1	−5·8827	−0·3313	−0·0011	—
5·0	1	0·0344	—	**5·0**	1	−6·0663	−0·3538	−0·0009	—
5·5	1	0·0351	—	**5·5**	1	−6·5225	−0·4114	−0·0007	—
6·0	1	0·0352	—	**6·0**	1	−6·9760	−0·4700	−0·0005	—
6·5	1	0·0351	—	**6·5**	1	−7·4281	−0·5291	−0·0003	—
7·0	1	0·0347	—	**7·0**	1	−7·8797	−0·5885	−0·0001	—
7·5	1	0·0342	—	**7·5**	1	−8·3318	−0·6475	−0·0000	—
8·0	1	0·0335	—	**8·0**	1	−8·7851	−0·7061	−0·0000	—
8·5	1	0·0328	—	**8·5**	1	−9·2403	−0·7640	−0·0000	—
9·0	1	0·0321	—	**9·0**	1	−9·6979	−0·8207	−0·0002	—
				9·5	1	−10·1580	−0·8762	−0·0003	—
				10·0	1	−10·6209	−0·9304	−0·0005	—

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

$3s\,\sigma_g$

R	g_0	g_1	g_2	g_3	g_4	g_5	g_6
0·0	1	−2·0000	1·0000	0·0000	0·0000	0·0000	0·0000
0·2	1	−2·2829	1·2956	0·0001	0·0000	0·0000	0·0000
0·4	1	−2·5805	1·6318	0·0015	0·0001	0·0001	0·0000
0·6	1	−2·8812	1·9964	0·0048	0·0003	0·0001	0·0000
0·8	1	−3·1810	2·3833	0·0107	0·0007	0·0001	0·0000
1·0	1	−3·4787	2·7906	0·0194	0·0010	0·0001	0·0000
1·2	1	−3·7739	3·2161	0·0313	0·0015	0·0002	0·0000
1·4	1	−4·0663	3·6591	0·0465	0·0019	0·0002	0·0000
1·6	1	−4·3561	4·1186	0·0652	0·0023	0·0003	0·0000
1·8	1	−4·6432	4·5942	0·0874	0·0027	0·0003	0·0001
2·0	1	−4·9277	5·0852	0·1132	0·0031	0·0003	0·0001
2·2	1	−5·2099	5·5913	0·1428	0·0034	0·0003	0·0001
2·4	1	−5·4898	6·1122	0·1760	0·0037	0·0003	0·0001
2·6	1	−5·7675	6·6477	0·2131	0·0039	0·0003	—
2·8	1	−6·0431	7·1973	0·2540	0·0040	0·0003	—
3·0	1	−6·3168	7·7610	0·2987	0·0041	0·0003	—
3·2	1	−6·5885	8·3383	0·3474	0·0042	0·0003	—
3·4	1	−6·8585	8·9291	0·3999	0·0042	0·0002	—
3·6	1	−7·1268	9·5338	0·4564	0·0041	0·0002	—
3·8	1	−7·3934	10·1514	0·5168	0·0040	0·0002	—
4·0	1	−7·6585	10·7825	0·5811	0·0038	0·0002	—
4·2	1	−7·9222	11·4265	0·6495	0·0036	0·0001	—
4·4	1	−8·1844	12·0836	0·7217	0·0034	0·0001	—
4·6	1	−8·4454	12·7536	0·7979	0·0032	0·0001	—
4·8	1	−8·7051	13·4366	0·8780	0·0029	0·0001	—
5·0	1	−8·9636	14·1324	0·9622	0·0027	0·0001	—
5·5	1	−9·6052	15·9280	1·1895	0·0020	0·0001	—
6·0	1	−10·2408	17·8039	1·4410	0·0012	0·0000	—
6·5	1	−10·8713	19·7601	1·7166	0·0006	0·0000	—
7·0	1	−11·4975	21·7977	2·0158	0·0001	0·0000	—
7·5	1	−12·1201	23·9174	2·3384	0·0000	0·0000	—
8·0	1	−12·7399	26·1206	2·6838	0·0003	0·0000	—
8·5	1	−13·3576	28·4089	3·0516	0·0010	0·0001	—
9·0	1	−13·9739	30·7845	3·4412	0·0021	0·0001	—
9·5	1	−14·5893	33·2490	3·8520	0·0038	0·0002	—
10·0	1	−15·2042	35·8043	4·2838	0·0063	0·0003	—

$2p\,\sigma_u$

R	g_0	g_1	g_2
0·0	1	1·0000	0·0000
0·2	1	0·8099	0·0000
0·4	1	0·6418	0·0001
0·6	1	0·4990	0·0002
0·8	1	0·3831	0·0003
1·0	1	0·2935	0·0005
1·2	1	0·2270	0·0006
1·4	1	0·1788	0·0006
1·6	1	0·1444	0·0006
1·8	1	0·1198	0·0006
2·0	1	0·1019	0·0005
2·2	1	0·0888	0·0005
2·4	1	0·0790	0·0004
2·6	1	0·0714	0·0004
2·8	1	0·0656	0·0004
3·0	1	0·0611	0·0004
3·2	1	0·0573	0·0003
3·4	1	0·0543	0·0002
3·6	1	0·0519	0·0002
3·8	1	0·0498	0·0002
4·0	1	0·0480	0·0002
4·2	1	0·0465	0·0002
4·4	1	0·0452	0·0002
4·6	1	0·0441	0·0002
4·8	1	0·0431	0·0001
5·0	1	0·0422	—
5·5	1	0·0403	—
6·0	1	0·0387	—
6·5	1	0·0374	—
7·0	1	0·0362	—
7·5	1	0·0351	—
8·0	1	0·0341	—
8·5	1	0·0331	—
9·0	1	0·0323	—

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

TABLE 3. THE COEFFICIENTS OF THE λ EXPANSION ((13) OF TEXT) (*cont.*)

	$3p\sigma_u$					$4p\sigma_u$						
R	g_0	g_1	g_2	g_3	g_4	R	g_0	g_1	g_2	g_3	g_4	g_5
0·0	1	0·0000	−1·0000	0·0000	0·0000	**0·0**	1	−1·0000	−1·0000	1·0000	0·0000	0·0000
0·2	1	−0·2593	−0·8662	−0·0000	−0·0000	**0·2**	1	−1·2935	−0·5984	0·8957	0·0000	0·0000
0·4	1	−0·5033	−0·7370	−0·0000	−0·0000	**0·4**	1	−1·5740	−0·2001	0·7891	0·0001	0·0000
0·6	1	−0·7316	−0·6205	−0·0002	−0·0000	**0·6**	1	−1·8420	+0·1865	0·6898	0·0002	0·0000
0·8	1	−0·9461	−0·5231	−0·0004	−0·0000	**0·8**	1	−2·1004	0·5576	0·6062	0·0004	0·0000
1·0	1	−1·1513	−0·4479	−0·0006	−0·0000	**1·0**	1	−2·3538	0·9158	0·5437	0·0007	0·0000
1·2	1	−1·3518	−0·3940	−0·0008	−0·0000	**1·2**	1	−2·6069	1·2685	0·5029	0·0009	0·0001
1·4	1	−1·5518	−0·3581	−0·0009	−0·0001	**1·4**	1	−2·8631	1·6243	0·4816	0·0011	0·0001
1·6	1	−1·7538	−0·3359	−0·0010	−0·0001	**1·6**	1	−3·1239	1·9904	0·4762	0·0012	0·0001
1·8	1	−1·9586	−0·3237	−0·0010	−0·0001	**1·8**	1	−3·3894	2·3713	0·4834	0·0013	0·0001
2·0	1	−2·1663	−0·3189	−0·0010	−0·0001	**2·0**	1	−3·6590	2·7697	0·5005	0·0013	0·0001
2·2	1	−2·3763	−0·3192	−0·0010	−0·0001	**2·2**	1	−3·9318	3·1866	0·5257	0·0013	0·0001
2·4	1	−2·5881	−0·3234	−0·0009	−0·0001	**2·4**	1	−4·2072	3·6227	0·5576	0·0013	0·0001
2·6	1	−2·8010	−0·3306	−0·0009	−0·0001	**2·6**	1	−4·4842	4·0780	0·5954	0·0012	0·0001
2·8	1	−3·0148	−0·3399	−0·0009	−0·0001	**2·8**	1	−4·7626	4·5525	0·6384	0·0012	0·0001
3·0	1	−3·2289	−0·3509	−0·0008	−0·0001	**3·0**	1	−5·0417	5·0458	0·6861	0·0011	0·0001
3·2	1	−3·4432	−0·3632	−0·0007	—	**3·2**	1	−5·3213	5·5580	0·7382	0·0010	0·0001
3·4	1	−3·6573	−0·3767	−0·0006	—	**3·4**	1	−5·6012	6·0887	0·7946	0·0009	0·0001
3·6	1	−3·8711	−0·3911	−0·0006	—	**3·6**	1	−5·8811	6·6378	0·8550	0·0008	—
3·8	1	−4·0845	−0·4063	−0·0005	—	**3·8**	1	−6·1609	7·2050	0·9192	0·0006	—
4·0	1	−4·2974	−0·4221	−0·0005	—	**4·0**	1	−6·4405	7·7903	0·9873	0·0005	—
4·2	1	−4·5097	−0·4384	−0·0004	—	**4·2**	1	−6·7197	8·3932	1·0591	0·0004	—
4·4	1	−4·7214	−0·4552	−0·0004	—	**4·4**	1	−6·9986	9·0138	1·1346	0·0003	—
4·6	1	−4·9325	−0·4724	−0·0003	—	**4·6**	1	−7·2771	9·6520	1·2137	0·0002	—
4·8	1	−5·1429	−0·4899	−0·0002	—	**4·8**	1	−7·5551	10·3075	1·2963	0·0001	—
5·0	1	−5·3526	−0·5076	−0·0001	—	**5·0**	1	−7·8326	10·9802	1·3825	0·0001	—
5·5	1	−5·8740	−0·5531	−0·0001	—	**5·5**	1	−8·5242	12·7369	1·6134	0·0000	—
6·0	1	−6·3914	−0·5997	0·0000	—	**6·0**	1	−9·2125	14·5991	1·8659	0·0001	—
6·5	1	−6·9050	−0·6470	0·0000	—	**6·5**	1	−9·8975	16·5657	2·1396	0·0004	—
7·0	1	−7·4152	−0·6946	0·0000	—	**7·0**	1	−10·5793	18·6355	2·4345	0·0010	—
7·5	1	−7·9223	−0·7425	0·0000	—	**7·5**	1	−11·2581	20·8081	2·7501	0·0019	—
8·0	1	−8·4267	−0·7903	−0·0001	—	**8·0**	1	−11·9339	23·0824	3·0863	0·0031	—
8·5	1	−8·9286	−0·8381	−0·0003	—	**8·5**	1	−12·6071	25·4580	3·4429	0·0049	—
9·0	1	−9·4286	−0·8854	−0·0005	—	**9·0**	1	−13·2778	27·9348	3·8195	0·0069	—
9·5	1	−9·9267	−0·9324	−0·0006	—	**9·5**	1	−13·9461	30·5124	4·2157	0·0094	—
10·0	1	−10·4234	−0·9786	−0·0007	—	**10·0**	1	−14·6123	33·1904	4·6317	0·0126	—

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	$3d\sigma_g$		
R	g_0	g_1	g_2
0·0	1	4·0000	1·0000
0·2	1	3·7362	0·8731
0·4	1	3·4785	0·7584
0·6	1	3·2270	0·6550
0·8	1	2·9823	0·5620
1·0	1	2·7446	0·4788
1·2	1	2·5147	0·4045
1·4	1	2·2933	0·3387
1·6	1	2·0810	0·2808
1·8	1	1·8788	0·2303
2·0	1	1·6878	0·1867
2·2	1	1·5089	0·1496
2·4	1	1·3431	0·1185
2·6	1	1·1914	0·0929
2·8	1	1·0543	0·0721
3·0	1	0·9321	0·0556
3·2	1	0·8247	0·0428
3·4	1	0·7313	0·0330
3·6	1	0·6510	0·0255
3·8	1	0·5826	0·0198
4·0	1	0·5247	0·0156
4·2	1	0·4759	0·0125
4·4	1	0·4348	0·0101
4·6	1	0·4002	0·0082
4·8	1	0·3711	0·0068
5·0	1	0·3467	0·0059
5·5	1	0·3010	0·0045
6·0	1	0·2707	0·0036
6·5	1	0·2505	0·0032
7·0	1	0·2370	0·0029
7·5	1	0·2280	0·0029
8·0	1	0·2221	0·0028
8·5	1	0·2184	0·0028
9·0	1	0·2164	0·0030
9·5	1	0·2155	0·0032
10·0	1	0·2153	0·0034

	$4f\sigma_u$			
R	g_0	g_1	g_2	g_3
0·0	1	9·0000	9·0000	1·0000
0·2	1	8·7015	8·4140	0·9039
0·4	1	8·4060	7·8557	0·8156
0·6	1	8·1135	7·3241	0·7343
0·8	1	7·8241	6·8185	0·6598
1·0	1	7·5379	6·3381	0·5914
1·2	1	7·2548	5·8821	0·5288
1·4	1	6·9751	5·4497	0·4717
1·6	1	6·6988	5·0403	0·4196
1·8	1	6·4259	4·6529	0·3723
2·0	1	6·1566	4·2870	0·3292
2·2	1	5·8910	3·9417	0·2903
2·4	1	5·6293	3·6163	0·2550
2·6	1	5·3715	3·3101	0·2232
2·8	1	5·1178	3·0225	0·1947
3·0	1	4·8685	2·7527	0·1690
3·2	1	4·6237	2·5002	0·1461
3·4	1	4·3836	2·2642	0·1257
3·6	1	4·1485	2·0442	0·1075
3·8	1	3·9188	1·8396	0·0915
4·0	1	3·6946	1·6499	0·0774
4·2	1	3·4763	1·4744	0·0650
4·4	1	3·2644	1·3127	0·0543
4·6	1	3·0592	1·1642	0·0450
4·8	1	2·8612	1·0286	0·0370
5·0	1	2·6708	0·9052	0·0303
5·5	1	2·2308	0·6466	0·0175
6·0	1	1·8473	0·4523	0·0096
6·5	1	1·5241	0·3123	0·0051
7·0	1	1·2605	0·2153	0·0026
7·5	1	1·0514	0·1501	0·0013
8·0	1	0·8889	0·1069	0·0007
8·5	1	0·7634	0·0783	0·0003
9·0	1	0·6666	0·0593	0·0001
9·5	1	0·5916	0·0465	—
10·0	1	0·5327	0·0373	—

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TABLE 3. THE COEFFICIENTS OF THE λ EXPANSION ((13) OF TEXT) (*cont.*)

	$2p\,\pi_u$			$3d\,\pi_g$			
R	g_0	g_1	g_2	R	g_0	g_1	g_2
0·0	1	0·0000	0·0000	**0·0**	1	1·0000	0·0000
0·2	1	0·0011	−0·0000	**0·2**	1	0·9351	−0·0000
0·4	1	0·0037	−0·0000	**0·4**	1	0·8734	−0·0001
0·6	1	0·0070	−0·0000	**0·6**	1	0·8152	−0·0004
0·8	1	0·0107	−0·0000	**0·8**	1	0·7606	−0·0006
1·0	1	0·0146	−0·0001	**1·0**	1	0·7095	−0·0008
1·2	1	0·0185	−0·0001	**1·2**	1	0·6620	−0·0010
1·4	1	0·0224	−0·0002	**1·4**	1	0·6179	−0·0011
1·6	1	0·0262	−0·0002	**1·6**	1	0·5772	−0·0012
1·8	1	0·0300	−0·0003	**1·8**	1	0·5398	−0·0013
2·0	1	0·0337	−0·0003	**2·0**	1	0·5056	−0·0014
2·2	1	0·0372	−0·0004	**2·2**	1	0·4744	−0·0014
2·4	1	0·0407	−0·0004	**2·4**	1	0·4460	−0·0014
2·6	1	0·0442	−0·0005	**2·6**	1	0·4202	−0·0014
2·8	1	0·0476	−0·0005	**2·8**	1	0·3968	−0·0014
3·0	1	0·0508	−0·0006	**3·0**	1	0·3757	−0·0013
3·2	1	0·0540	−0·0006	**3·2**	1	0·3566	−0·0013
3·4	1	0·0572	−0·0007	**3·4**	1	0·3393	−0·0012
3·6	1	0·0602	−0·0007	**3·6**	1	0·3238	−0·0012
3·8	1	0·0632	−0·0007	**3·8**	1	0·3097	−0·0011
4·0	1	0·0662	−0·0008	**4·0**	1	0·2970	−0·0010
4·2	1	0·0690	−0·0008	**4·2**	1	0·2855	−0·0010
4·4	1	0·0718	−0·0008	**4·4**	1	0·2752	−0·0009
4·6	1	0·0746	−0·0009	**4·6**	1	0·2658	−0·0008
4·8	1	0·0772	−0·0009	**4·8**	1	0·2572	−0·0008
5·0	1	0·0799	−0·0009	**5·0**	1	0·2495	−0·0007
5·5	1	0·0861	−0·0010	**5·5**	1	0·2331	−0·0005
6·0	1	0·0921	−0·0009	**6·0**	1	0·2200	−0·0004
6·5	1	0·0978	−0·0008	**6·5**	1	0·2095	−0·0002
7·0	1	0·1030	−0·0008	**7·0**	1	0·2010	−0·0001
7·5	1	0·1080	−0·0008	**7·5**	1	0·1940	0·0000
8·0	1	0·1126	−0·0007	**8·0**	1	0·1883	+0·0002
8·5	1	0·1170	−0·0006	**8·5**	1	0·1835	0·0003
9·0	1	0·1210	−0·0004	**9·0**	1	0·1794	0·0004
9·5	1	0·1247	−0·0004	**9·5**	1	0·1759	0·0004
10·0	1	0·1281	−0·0003	**10·0**	1	0·1729	0·0005