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Three-Term Hylleraas-Function Atomic Scattering Factors for the Two-Electron Ions*

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The three term Hylleraas function $\psi=[1+c_1u+c_2t^2]\exp(-\alpha s)$ is used to determine the atomic scattering factors for the helium-like ions. Though some systematic differences are noted, previous self-consistent field and radially correlated factors are found to be in good agreement with present results. It is found that the radial correlation introduced by use of the so-called 'open shell' approximation tends to slightly overemphasize the correlation effect. When one introduces angular correlation as well, the shift in the radial distribution is slightly reduced. Finally, it is noted that the scattering factors from the Hylleraas function tend to be smaller than those computed from hydrogenic charge distributions (hydrogenic charge distribution with a scale factor) at small Bragg angles and larger at the large Bragg angles. An explanation for this latter effect is given.

1. Introduction

Of the many variational functions proposed to describe the electronic ground state of helium and helium-like ions, the famous function developed by Hylleraas (1929) is still considered to be one of the most successful (see, for example, Bethe & Salpeter (1957)) for obtaining electronic energies. As such, the Hylleraas function, essentially an expansion in terms of the relative position of the electrons from each other and from the nucleus, has been of considerable interest for computing observables other than the energy.

In the present paper, atomic form factors are obtained from the singlet-state three-term Hylleraas function

$$\psi=\exp[-\alpha s][1+c_1u+c_2t^2]A(1,2)\,, \qquad (1a)$$

where

$$s=r_1+r_2 \qquad (1b)$$

$$u=r_{12} \qquad (1c)$$

$$t=r_2-r_1 \qquad (1d)$$

and where

$$A(1,2)=(1/\sqrt{2})[\alpha(1)\beta(2)-\alpha(2)\beta(1)]\,, \qquad (1e)$$

i.e., $A(1,2)$ is the antisymmetric spin function. Here the normalization factor has been omitted.

Since this wave function gives lower calculated energies than can be computed from the wave functions used for previous form-factor calculations, one can reasonably hope to obtain improved factors. However, as Ibers (1959) has recently emphasized, the wave function yielding the lowest energy need not necessarily give the most reliable form factors. Thus, though experience has shown the energy criterion to be generally useful, conclusions based upon it should be accepted with some reservations. A more detailed discussion of this problem is given elsewhere (Silverman, Platas & Matsen, 1959).

2. Theory

The form factors f are obtained from (see James (1948))

$$f=\frac{\int\psi\left(\sum_{k=1}^{2}\exp[i\mu r_k\cos\theta_k]\right)\psi d\tau}{N}\,, \qquad (2a)$$

where

$$\mu=4\pi\sin(\theta)/\lambda \qquad (2b)$$

and

$$N=\int\psi\psi d\tau\,. \qquad (2c)$$

In this case, and henceforth, the Bragg angle θ is distinguished from the co-latitude angle of the kth electron by the subscript k and λ is the wavelength of the X-ray beam.

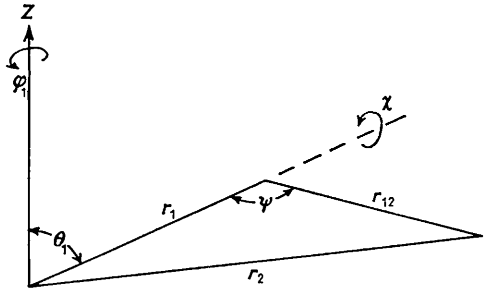

Fig. 1.

Upon substituting equations (1) into (2), one obtains after integrating out the spin coordinates

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$$f=(1/N)[k_{0,0}(\mu,\alpha)+2c_1k_{0,1}(\mu,\alpha)+2c_2k_{2,0}(\mu,\alpha)$$
$$+c_1^2k_{0,2}(\mu,\alpha)+2c_1c_2k_{2,1}(\mu,\alpha)+c_2^2k_{4,0}(\mu,\alpha)]\ , \quad (3a)$$

where

$$k_{l,m}(\mu,\alpha)=2\int\exp\left[-2\alpha s+i\mu r_1\cos\theta_1\right]t^lu^md\tau\ . \quad (3b)$$

In order to complete the analysis one must devise a method of evaluating the auxiliary functions $k_{l,m}(\mu,\alpha)$. Since the integrand of this function contains the interelectronic distance r_{12} explicitly, one should attempt to find a two-electron coordinate system. Such a system is suggested by Margenau & Murphy (1943). Then, following these authors, the volume element becomes (see Fig. 1)

$$d\tau=r_1^2dr_1\sin\theta_1d\theta_1r_{12}^2dr_{12}\sin\psi d\psi d\chi d\varphi_1\ . \quad (4)$$

Since

$$r_2^2=r_1^2+r_{12}^2-2r_1r_{12}\cos\psi \quad (5)$$

we have

$$r_2dr_2=r_1r_{12}\sin\psi d\psi \quad (6)$$

so that $d\tau$ becomes

$$d\tau=r_1dr_1r_2dr_2r_{12}dr_{12}\sin\theta_1d\theta_1d\chi d\varphi_1\ . \quad (7)$$

Here the limits of the integration are

$$|r_1-r_2|\le r_{12}\le r_1+r_2 \quad (8a)$$
$$0\le r_1<\infty \quad (8b)$$
$$0\le r_2<\infty \quad (8c)$$
$$0\le\theta_1\le\pi \quad (8d)$$
$$0\le\varphi_1\le 2\pi \quad (8e)$$
$$0\le\chi\le 2\pi\ . \quad (8f)$$

Since the integrand does not contain φ_1 or χ, integration over these angles reduces the volume element to

$$d\tau=4\pi^2r_1dr_1r_2dr_2r_{12}dr_{12}\sin\theta_1d\theta_1\ . \quad (9)$$

Then after integrating over θ_1 we have

$$k_{l,m}(\mu,\alpha)=\frac{16\pi^2}{\mu}\left(\int_0^\infty\exp\left[-2\alpha r_1\right]\sin\mu r_1dr_1\right.$$
$$\times\int_{r_1}^\infty\exp\left[-2\alpha r_2\right]r_2dr_2\int_t^s t^lu^{m+1}du$$
$$+\int_{r_2}^\infty\exp\left[-2\alpha r_1\right]\sin\mu r_1dr_1$$
$$\left.\times\int_0^\infty\exp\left[-2\alpha r_2\right]r_2dr_2\int_{-t}^s t^lu^{m+1}du\right)\ , \quad (10)$$

Equation (10) is then evaluated by successive application of the general identity

$$\int_0^\infty h(x)dx\int_x^\infty j(y)dy+\int_0^\infty j(x)dx\int_x^\infty h(y)dy=H(0)J(0) \quad (11a)$$

where we define

$$\int_0^\infty h(y)dy=-H(0) \quad (11b)$$

and

$$\int_0^\infty j(y)dy=-J(0)\ . \quad (11c)$$

To show how this procedure works, we consider two examples which illustrate the special cases $m=2n$ (even) and $m=2n+1$ (odd). Selecting an example of the first case, we have

$$k_{0,0}(\mu,\alpha)=\frac{16\pi^2}{\mu}\left(\int_0^\infty(\exp\left[-2\alpha r_1\right]\sin\mu r_1dr_1\right.$$
$$\times\int_{r_1}^\infty\exp\left[-2\alpha r_2\right]r_2dr_2\int_t^s u\,du$$
$$+\int_{r_2}^\infty\exp\left[-2\alpha r_1\right]\sin\mu r_1dr_1$$
$$\left.\times\int_0^\infty\exp\left[-2\alpha r_2\right]r_2dr_2\int_{-t}^s u\,du\right) \quad (12)$$

$$k_{0,0}(\mu,\alpha)=\frac{16\pi^2}{\mu}\left(2\int_0^\infty\exp\left[-2\alpha r_1\right]r_1\sin\mu r_1dr_1\right.$$
$$\times\int_{r_1}^\infty\exp\left[-2\alpha r_2\right]r_2^2dr_2$$
$$+2\int_{r_2}^\infty\exp\left[-2\alpha r_1\right]r_1\sin\mu r_1dr_1$$
$$\left.\times\int_0^\infty\exp\left[-2\alpha r_2\right]r_2^2dr_2\right)\ . \quad (13)$$

Then, upon applying equations (11), one obtains

$$k_{0,0}(\mu,\alpha)=16\pi^2[2g_1(\alpha,\mu)h_2(\alpha)]\ , \quad (14)$$

where we define

$$g_n(\alpha,\mu)=\frac{1}{\mu}\int_0^\infty\exp\left[-2\alpha r_1\right]r_1^n\sin\mu r_1dr_1$$
$$=\frac{Im}{\mu}\left(\frac{(2\alpha+i\mu)^{n+1}}{(4\alpha^2+\mu^2)^{n+1}}n!\right) \quad (15)$$

and

$$h_n(\alpha)=\int_0^\infty\exp\left[-2\alpha r_1\right]r_1^ndr_1=\frac{n!}{(2\alpha)}n+1\ . \quad (16)$$

To illustrate the second case (m odd), $k_{0,1}(\mu,\alpha)$ becomes, after integrating over u and substituting in the limits,

$$k_{0,1}(\mu,\alpha)=\frac{16\pi^2}{3\mu}\left[\int_0^\infty\exp\left[-2\alpha r_1\right]\sin\mu r_1dr_1\right.$$
$$\times\int_{r_1}^\infty\exp\left[-2\alpha r_2\right]r_2dr_2(6r_2^2r_1+2r_1^3)$$
$$+\int_0^\infty\exp\left[-2\alpha r_2\right]r_2dr_2\int_{r_2}^\infty\exp\left[-2\alpha r_1\right]$$
$$\left.\times\sin\mu r_1dr_1(6r_1^2r_2+2r_2^3)\right]\ . \quad (17)$$

Then equations (11) can be applied, if equation (17) is written

$$\begin{aligned}k_{0,1}(\mu,\alpha) = \frac{16\pi^2}{3\mu}\Bigg[&\int_0^\infty \exp\,[-2\alpha r_1]\sin\mu r_1 dr_1\\ &\times\int_{r_1}^\infty \exp\,[-2\alpha r_2]r_2dr_2(6r_2^2r_1+2r_1^3)\\ &-\int_0^\infty \exp\,[-2\alpha r_2]\sin\mu r_2dr_2\\ &\times\int_{r_2}^\infty \exp\,[-2\alpha r_1]r_1dr_1(6r_1r_2^2+2r_1^3)\\ &+\int_0^\infty \exp\,[-2\alpha r_2]\sin\mu r_2dr_2\\ &\times\int_{r_2}^\infty \exp\,[-2\alpha r_1]r_1dr_1(6r_1r_2^2+2r_1^3)\\ &+\int_0^\infty \exp\,[-2\alpha r_2]r_2dr_2\\ &\times\int_{r_2}^\infty \exp\,[-2\alpha r_1]\sin\mu r_1dr_1(6r_1^2r_2+2r_2^3)\Bigg].\end{aligned} \tag{18}$$

The first two terms of the right side of equation (18) are easily reduced using the general result

$$\begin{aligned}\int_{r_1}^\infty \exp\,[-2\alpha r_2]r_2^ndr_2 = \exp\,[-2\alpha r_1][&h_0(\alpha)r_1^n\\ &+nh_1(\alpha)r_1^{n-1}+\frac{n(n-1)}{2!}h_2(\alpha)r_1^{n-2}+\ldots]\end{aligned} \tag{19}$$

so that after applying equations (11) and (19), one obtains

$$\begin{aligned}k_{0,1}(\mu,\alpha)=16\pi^2[&2g_2(\alpha,\mu)h_2(\alpha)+2/3g_0(\alpha,\mu)h_4(\alpha)\\ &-2/3g_1(2\alpha,\mu)h_3(\alpha)-2/3g_0(2\alpha,\mu)h_4(\alpha)]\,.\end{aligned} \tag{20}$$

Table 1. *Scattering integral formulae*
(Atomic units)

(*a*) $k_{0,0}(\mu,\alpha) = 16\pi^2[2g_1(\alpha,\mu)h_2(\alpha)]$

(*b*) $k_{0,1}(\mu,\alpha) = 16\pi^2[2g_2(\alpha,\mu)h_2(\alpha)+2/3g_0(\alpha,\mu)h_4(\alpha)-2/3g_1(2\alpha,\mu)h_3(\alpha)-2/3g_0(2\alpha,\mu)h_4(\alpha)]$

(*c*) $k_{2,0}(\mu,\alpha) = 16\pi^2[2g_3(\alpha,\mu)h_2(\alpha)-4g_2(\alpha,\mu)h_3(\alpha)+2g_1(\alpha,\mu)h_4(\alpha)]$

(*d*) $k_{0,2}(\mu,\alpha) = 16\pi^2[2g_3(\alpha,\mu)h_2(\alpha)+2g_1(\alpha,\mu)h_4(\alpha)]$

(*e*) $k_{2,1}(\mu,\alpha) = 16\pi^2[2g_4(\alpha,\mu)h_2(\alpha)-4g_3(\alpha,\mu)h_3(\alpha)+8/3g_2(\alpha,\mu)h_4(\alpha)-4/3g_1(\alpha,\mu)h_5(\alpha)+2/3g_0(\alpha,\mu)h_6(\alpha)-2/3g_1(2\alpha,\mu)h_5(\alpha)-2/3g_0(2\alpha,\mu)h_6(\alpha)]$

(*f*) $k_{4,0}(\mu,\alpha) = 16\pi^2[2g_5(\alpha,\mu)h_2(\alpha)-8g_4(\alpha,\mu)h_3(\alpha)+12g_3(\alpha,\mu)h_4(\alpha)-8g_2(\alpha,\mu)h_5(\alpha)+2g_1(\alpha,\mu)h_6(\alpha)]$

(*g*) $g_n(\alpha,\mu) = 1/\mu\int_0^\infty \exp\,[-2\alpha r]r^n\sin\mu r\,dr = \frac{Im}{\mu}\left(\frac{(2\alpha+i\mu)^{n+1}n!}{(4\alpha^2+\mu^2)^{n+1}}\right)$

(*h*) $h_n(\alpha) = \int_0^\infty \exp\,[-2\alpha r]r^ndr = \frac{n!}{(2\alpha)^{n+1}}$

The remaining integrals are evaluated by the same techniques and are collected in Table 1. No new formulae are required to evaluate the normalization integral N (cf. equations (2)) as this is obtained from equations (3) using the relation $f=2$ at $\mu=0$.

Finally, to summarize, the atomic scattering factors are obtained from equations (3) using the functions $k_{l,m}(\mu,\alpha)$ listed in Table 1. The parameters α, c_1 and c_2 are accurately refined but are not given here as they are listed elsewhere*. Finally, all calculations are performed on a Bendix G-15 D computer using 12-place arithmetic.

Table 2. *Three term Hylleraas function atomic scattering factors for helium-like ions*

$\sin\theta/\lambda$ Å^{-1}	H$^-$	He	Li$^+$	Be^{++}
0·000	2·0000	2·0000	2·0000	2·0000
0·025	1·9212	1·9892	1·9959	1·9979
0·050	1·7148	1·9573	1·9837	1·9915
0·075	1·4485	1·9060	1·9636	1·9809
0·100	1·1847	1·8378	1·9361	1·9663
0·125	0·95745	1·7558	1·9015	1·9477
0·150	0·77441	1·6634	1·8606	1·9253
0·175	0·63038	1·5642	1·8141	1·8995
0·200	0·51691	1·4612	1·7626	1·8703
0·225	0·42661	1·3573	1·7071	1·8380
0·250	0·35396	1·2548	1·6482	1·8030
0·275	0·29500	1·1555	1·5868	1·7655
0·300	0·24685	1·0607	1·5237	1·7258
0·325	0·20736	0·97121	1·4594	1·6843
0·350	0·17484	0·88764	1·3948	1·6411
0·375	0·14798	0·81016	1·3302	1·5967
0·400	0·12572	0·73877	1·2663	1·5512
0·425	0·10722	0·67330	1·2035	1·5050
0·450	0·09179	0·61349	1·1421	1·4583
0·475	0·07888	0·55901	1·0824	1·4113
0·500	0·06804	0·50949	1·0246	1·3644
0·525	0·05890	0·46455	0·96892	1·3175
0·550	0·05118	0·42382	0·91550	1·2711
0·575	0·04462	0·38692	0·86439	1·2252
0·600	0·03904	0·35351	0·81563	1·1799
0·625	0·03427	0·32325	0·76924	1·1354
0·650	0·03018	0·29586	0·72521	1·0919
0·675	0·02667	0·27104	0·68348	1·0493
0·700	0·02363	0·24855	0·64402	1·0077
0·725	0·02100	0·22816	0·60674	0·96734
0·750	0·01872	0·20966	0·57159	0·92811
0·775	0·01672	0·19286	0·53846	0·89009
0·800	0·01499	0·17759	0·50728	0·85330
0·825	0·01346	0·16370	0·47795	0·81775
0·850	0·01212	0·15106	0·45037	0·78345
0·875	0·01094	0·13955	0·42447	0·75039
0·900	0·009896	0·12904	0·40014	0·71858
0·925	0·008971	0·11945	0·37731	0·68799
0·950	0·008150	0·11069	0·35587	0·65861
0·975	0·007419	0·10267	0·33576	0·63041
1·000	0·006767	0·09533	0·31688	0·60337
1·050	0·005661	0·08243	0·28256	0·55263
1·100	0·004769	0·07155	0·25233	0·50615
1·150	0·004043	0·06234	0·22570	0·46364
1·200	0·003449	0·05451	0·20221	0·42482
1·250	0·002959	0·04782	0·18149	0·38942
1·300	0·002552	0·04210	0·16317	0·35715
1·350	0·002212	0·03719	0·14695	0·32775
1·400	0·001927	0·03294	0·13259	0·30099
1·450	0·001685	0·02927	0·11984	0·27661
1·500	0·001480	0·02609	0·10850	0·25442

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* These results will be supplied upont request.

Table 3. *Atomic scattering factors for one, two, and three term Hylleraas functions*

$\sin\theta/\lambda$ Å^{-1} Ion	0·0	0·1	0·2	0·3	0·4	0·5	0·6	0·7	0·8	0·9	1·0	1·5	Number of terms in fcn.
H^-	2·000	1·314	0·5339	0·2074	0·0889	0·0427	0·0225	0·0129	0·0078	0·0050	0·0034	0·00070	1
	2·000	1·313	0·5348	0·2147	0·0970	0·0489	0·0270	0·0159	0·0099	0·0065	0·0044	0·00094	2
	2·000	1·185	0·5169	0·2469	0·1257	0·0680	0·0390	0·0236	0·0150	0·0099	0·0068	0·0015	3
He	2·000	1·853	1·498	1·098	0·7610	0·5151	0·3479	0·2374	0·1647	0·1164	0·0839	0·0211	1
	2·000	1·850	1·490	1·088	0·7531	0·5113	0·3478	0·2398	0·1683	0·1204	0·0878	0·0231	2
	2·000	1·838	1·461	1·061	0·7388	0·5095	0·3535	0·2486	0·1776	0·1290	0·0953	0·0261	3
Li^+	2·000	1·940	1·776	1·545	1·291	1·046	0·8314	0·6531	0·5104	0·3987	0·3123	0·1013	1
	2·000	1·939	1·772	1·538	1·282	1·038	0·8246	0·6483	0·5077	0·3978	0·3129	0·1041	2
	2·000	1·936	1·763	1·524	1·266	1·025	0·8156	0·6440	0·5073	0·4001	0·3169	0·1085	3

Table 4. *Comparison of atomic scattering factors for helium-like ions*

$\sin\theta/\lambda$ Å^{-1} Ion	0·00	0·10	0·20	0·30	0·40	0·50	0·60	0·70	0·80	0·90	1·00	1·10	Electron distribution used
H^-	2·000	1·314	0·534	0·207	0·0889	0·0427	0·0225	0·0129	0·0078	0·0050	0·0034	0·0023	E
	2·000	1·064	0·519	0·255	0·130	0·0698	0·0398	0·0239	0·0151	0·0099	0·0068	0·0048	R
	2·000	1·185	0·517	0·247	0·126	0·0680	0·0390	0·0236	0·0150	0·0099	0·0068	0·0048	HY
He	2·000	1·853	1·498	1·098	0·761	0·515	0·348	0·237	0·165	0·116	0·084	0·062	E
	2·000	1·88	1·46	1·05	0·75	0·52	0·35	0·24	0·18	0·14	0·11	0·09	J&B
	2·000	1·832	1·452	1·058	0·742	0·515	0·358	0·251	0·179	0·129	0·0950	0·0709	R
	2·000	1·838	1·461	1·061	0·739	0·509	0·354	0·249	0·178	0·129	0·0953	0·0715	HY
Li^+	2·000	1·940	1·776	1·545	1·291	1·046	0·831	0·653	0·510	0·399	0·312	0·246	E
	2·000	1·936	1·762	1·522	1·264	1·022	0·813	0·642	0·505	0·398	0·316	0·252	F
	2·000	1·935	1·760	1·521	1·265	1·025	0·818	0·647	0·510	0·403	0·319	0·254	R
	2·000	1·936	1·763	1·524	1·266	1·025	0·816	0·644	0·507	0·400	0·317	0·252	HY
Be^{++}	2·000	1·968	1·876	1·737	1·566	1·381	1·197	1·023	0·865		0·608		E
	2·000	2·0	1·9	1·7	1·6	1·4	1·2	1·0	0·9	0·7	0·6	0·5	I
	2·000	1·966	1·869	1·724	1·550	1·363	1·180	1·009	0·855	0·721	0·606	0·508	R
	2·000	1·966	1·870	1·726	1·551	1·364	1·180	1·008	0·853	0·719	0·603	0·506	HY
B^{+++}	2·000	1·980	1·922	1·830	1·713	1·578	1·434	1·287	1·144		0·885		E
	2·000	1·99	1·9	1·8	1·7	1·6	1·4	1·3	1·2		0·9		I
	2·000	1·979	1·919	1·824	1·703	1·566	1·420	1·274	1·132		0·877		R
	2·000	1·979	1·919	1·825	1·704	1·567	1·421	1·274	1·132	0·998	0·876	0·765	HY
C^{+4}	2·000	1·986	1·946	1·882	1·798	1·698	1·586	1·467	1·347		1·111		E
	2·000	1·986	1·945	1·880	1·794	1·692	1·579	1·459	1·338	1·219	1·104	0·994	F
	2·000	1·986	1·945	1·879	1·972	1·689	1·576	1·457	1·335		1·101		R
	2·000	1·986	1·945	1·879	1·792	1·690	1·577	1·457	1·336	1·216	1·101	0·992	HY
N^{+5}	2·000	1·990	1·960	1·912	1·847	1·769	1·680	1·583	1·482	1·379	1·276	1·176	HY
O^{+5}	2·000	1·992	1·970	1·933	1·883	1·822	1·751	1·672	1·588	1·501	1·411	1·322	HY
F^{+7}	2·000	1·994	1·976	1·947	1·908	1·859	1·801	1·737	1·667	1·592	1·515	1·436	HY
Ne^{+8}	2·000	1·995	1·981	1·957	1·925	1·885	1·838	1·784	1·725	1·662	1·595	1·526	HY

E = Product of exponentials, i.e. $\psi = N_{1s}^2 \exp[-\alpha(r_1+r_2)]$. R = Radially correlated (Hurst, Miller & Matsen, 1958).
HY = Three term Hylleraas fcn. J&B = Hartree distribution (James & Brindley, 1931).
F = Hartree distribution (Freeman, 1958). I = Interpolated from Hartree distribution (James & Brindley, 1931).

3. Results

In Table 2 are given the three term Hylleraas function scattering factors for H^-, He, Li^+ and Be^{++} for rather small increments over most of the range; i.e.,

$$0 \leq (\sin\theta/\lambda) \leq 1·5\,.$$

One-, two- and three-term Hylleraas-function factor results are compared for H^-, He, and Li^+ in Table 3. In each case these calculations were made with optimized parameters; that is, for example, the optimized parameters α and c_1 required to determine the two-term results were obtained from variational calculations subject to the condition $C_2 = 0$.

Finally, in Table 4 the present three-term results are compared with the factors obtained for a number of previous calculations.

4. Discussion

Because the Hylleraas-type wavefunction, with r_{12} terms included explicitly in the numerator, is exceedingly difficult to extend to systems with more than two electrons, one should regard the present work principally as an attempt to obtain some indication of the accuracy of presently available atomic form factors. Both the Hartree-type factors (Freeman, 1958) and the radially correlated factors (Hurst, Miller & Matsen, 1958) are in good agreement with results from the three-term Hylleraas function. From inspection of Table 4 for C^{+4} the radially correlated factors deviate from the Hylleraas factors by at most 0·001 electrons while the Hartree factors deviate from the Hylleraas factors by at most 0·003 electrons. For Li^+ the maximum deviations from the Hylleraas factors are 0·003 electrons for both the radially correlated and Hartree results. The James & Brindley (1931) results are not given to sufficient accuracy to make this type of comparison meaningful.

The effect of using a better 'correlated' wavefunction is to increase the size of the atomic scattering factor at large values of $\sin\theta/\lambda$ and reduce its size at the smaller arguments. Thus from Table 3 one notes that for each of the three ions H^-, He and Li^+ at $\sin\theta/\lambda=1\cdot5$ the magnitude of the form factors lie in the order

$$\text{one term function} < \text{two term function} < \text{three term function}.$$

For $\sin\theta/\lambda=0\cdot1$ the order is reversed.

This effect is explained from the nature of the scattering operator (see, for example, Hurst, Miller & Matsen, 1958). As f can be written as a Fourier transform of the charge distribution, variations in the inner regions of charge distribution affect mainly the outer region of f and vice versa. Then, since the hydrogenic charge distribution (one-term Hylleraas function) is too small at very small radial distances (see Bethe & Salpeter, 1957), the corresponding factors are too small at large arguments. Further, since the hydrogenic charge distribution is always positive and is normalized, if it is too small at small radial distances it must be too large at some larger radial distances and the effect is reflected in the form factors at small arguments.

Finally, though as we have already emphasized that the radially correlated factors (Hurst, Miller & Matsen, 1958) are in quite good agreement with those computed from the Hylleraas function, there is an interesting systematic deviation. In Table 4 one notes in most cases for small atomic numbers and at large values of the argument $\sin\theta/\lambda$ that the radially correlated factors are slightly larger than the Hylleraas factor and that the Hylleraas factors are larger than the hydrogenic wavefunction factors. This could be explained by the facts that introducing radial correlation alone tends to overcompensate for the correlation effect and that when one introduces angular correlation as well by including an r_{12} term in the wavefunction the shift in the radial distribution is slightly reduced. A similar effect is found when a $(2p)^2$ configuration is introduced into the radially correlated wavefunction (Silverman, Platas & Matsen, 1959).

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