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Expansion coefficients and moments of electron momentum densities for singly charged ions

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Abstract. Numerical Hartree–Fock calculations of the first three coefficients of the MacLaurin expansion and the leading coefficient of the large-p asymptotic expansion of the electron momentum densities $\Pi(p)$ are reported for 54 singly charged atomic cations from He$^+$ (atomic number $Z=2$) to Cs$^+$ ($Z=55$) and 43 anions from H$^-$ ($Z=1$) to I$^-$ ($Z=53$) in their experimental ground states. We also report all the finite moments $\langle p^k \rangle$ ($-2 \le k \le +4$) of the momentum densities $\Pi(p)$ for the above-mentioned 97 ionic species. The results are compared with the previous ones for neutral atoms [Koga and Thakkar (1996) J Phys B 29: 2973], and the dependence of the expansion coefficients and moments on nuclear charge is discussed among isoelectronic species.

Key words: Momentum density – Expansion coefficients – Moments – Singly charged ions

1 Introduction and definitions

The spherical average $\Pi(p)$ of the electron momentum density is defined by

$$\Pi(p) \equiv (4\pi)^{-1} \int \mathrm{d}\Omega_p \int \mathrm{d}\sigma\, \mathrm{d}\mathbf{y}_2 \cdots \mathrm{d}\mathbf{y}_N |\Phi(\mathbf{y}, \mathbf{y}_2, \ldots, \mathbf{y}_N)|^2 \;, \tag{1}$$

where $\Phi(\mathbf{y}_1, \ldots, \mathbf{y}_N)$ is the momentum wave function of an N-electron system, $\mathbf{y}_j \equiv (\mathbf{p}_j, \sigma_j)$ is the combined momentum-spin coordinate of the jth electron, and (p, Ω_p) with $\Omega_p \equiv (\theta_p, \phi_p)$ are spherical polar coordinates of the momentum vector $\mathbf{p}$.

The MacLaurin expansion of the momentum density $\Pi(p)$ reads [1–3]

$$\Pi(p) = \Pi(0) + \frac{\Pi^{ii}(0)}{2!}p^2 + \frac{\Pi^{iv}(0)}{4!}p^4 + O(p^6) \;. \tag{2a}$$

The expansion coefficients on the right-hand side of Eq. (2a), together with the moment $\langle p^{-1} \rangle$, also determine [1–3] the MacLaurin expansion of the isotropic Compton profile $J(q)$,

$$J(q) = \frac{\langle p^{-1} \rangle}{2} - \pi\Pi(0)q^2 - \frac{\pi\, \Pi^{ii}(0)}{4}q^4 - \frac{\pi\, \Pi^{iv}(0)}{72}q^6 + O(q^8) \;, \tag{2b}$$

where $J(q)$ is given within the impulse approximation by

$$J(q) = 2\pi \int_{|q|}^{\infty} \mathrm{d}p\, p\Pi(p) \;, \tag{3}$$

which also implies $\mathrm{d}J(q)/\mathrm{d}q = -2\pi q\, \Pi(q)$. Thus, it was suggested [4] that the first two coefficients $\Pi(0)$ and $\Pi^{ii}(0)/2!$ in Eq. (2a) should be extracted from experimental Compton profiles, because the experimental measurements are most accurate around the profile peak. The asymptotic large-p expansion of $\Pi(p)$ is given by [1–3]

$$\Pi(p) = b_8 Z^5 p^{-8} + O(p^{-10}) \;, \tag{4a}$$

where Z denotes atomic number. The corresponding expansion of the isotropic Compton profile $J(q)$ is [1–3]

$$J(q) = \frac{\pi b_8 Z^5}{3} q^{-6} + O(q^{-8}) \;, \tag{4b}$$

and the coefficient b_8 is important [5] for attempts to obtain the momentum moments $\langle p^k \rangle$ from experimental Compton profiles.

The momentum density $\Pi(p)$ is associated with the moments $\langle p^k \rangle$ defined by

$$\langle p^k \rangle \equiv 4\pi \int_0^{\infty} \mathrm{d}p\, p^{k+2}\Pi(p), \quad -2 \le k \le +4 \;, \tag{5}$$

where the limits on k are due to positive finiteness at $p=0$ and p^{-8} decay at large p of $\Pi(p)$ [1, 2, 6]. A special case of Eq. (5) for $k=0$ implies that our normalization is $\langle p^0 \rangle = \langle 1 \rangle = N$, the number of electrons. Many

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physical properties are connected to the momentum moments as reviewed in Refs. [1, 6–10]. For example, $\langle p^{-1}\rangle$ is twice the peak value $J(0)$ of the Compton profile $J(q)$, $\langle p\rangle/\pi$ is close [11] to the Slater–Dirac exchange energy, $\langle p^2\rangle$ is twice the nonrelativistic electronic kinetic energy, $\langle p^3\rangle$ is approximately proportional [11, 12] to the initial value of the Patterson function in X-ray crystallography, and $\langle p^4\rangle$ determines [13] the Breit–Pauli mass–velocity correction in quasirelativistic quantum theory. We note that for $0 \leq k \leq +4$ [1, 14, 15],

$$\langle p^k\rangle = 2(k+1)\langle q^k\rangle \ , \tag{6}$$

where $\langle q^k\rangle$ is a moment of the Compton profile,

$$\langle q^k\rangle \equiv \int_0^\infty \mathrm{d}q\, q^k J(q) \ , \tag{7a}$$

and [5]

$$\langle p^{-2}\rangle = 2\int_0^\infty \mathrm{d}q\, q^{-2}[J(0) - J(q)] \ . \tag{7b}$$

The physical reasons outlined above led to the study of the MacLaurin and asymptotic large-p expansion coefficients by Thakkar et al. [3] and Westgate et al. [9]. Extensive tabulations of the momentum moments $\langle p^k\rangle$ were also reported for neutral atoms by Ponce [16], Gadre et al. [17], Westgate et al. [9], and Garcia de la Vega and Miguel [18–21]. Unfortunately, all these previous tables are based on Roothaan–Hartree–Fock wave functions of Clementi and Roetti [22] and McLean and McLean [23], which are now known [24–28] to suffer from nontrivial errors and inaccuracies. It is only recently [10] that accurate Hartree–Fock values of the first three coefficients of the MacLaurin expansion, the leading coefficient of the large-p asymptotic expansion, and the moments $\langle p^k\rangle$ of $\Pi(p)$ have become available for all 103 neutral atoms from H ($Z = 1$) to Lr ($Z = 103$).

For singly charged atomic cations and anions, however, only two studies have been reported. Thakkar et al. [3] gave the MacLaurin and large-p expansion coefficients of $\Pi(p)$ based on the Clementi–Roetti [22] and McLean–McLean [23] wave functions. Gadre et al. [17] tabulated the momentum moments based on the Clementi–Roetti wave functions [22]; however, the Clementi–Roetti functions for anions were pointed out [26, 28] to be extremely poor, and the reliability of the results based on them remains in question. In the present paper, we therefore report tables of accurate Hartree–Fock values of the expansion coefficients and moments of the electron momentum density $\Pi(p)$ for the experimental ground states of 97 singly charged ions with fewer than 55 electrons ($N < 55$), i.e., 54 cations from He$^+$ ($Z = 2$) to Cs$^+$ ($Z = 55$) and 43 anions from H$^-$ ($Z = 1$) to I$^-$ ($Z = 53$). As in our previous work [10], we remove basis-set artifacts by using numerical Hartree–Fock wave functions to construct electron momentum densities for all the atomic ions. The present results together with the previous ones for neutral atoms [10] provide a compilation of accurate Hartree–Fock values, which will be useful as a reference in the study of atoms and molecules in momentum space. Hartree atomic units are used throughout this paper.

2 Computational method

For the singly charged cations He$^+$ to Cs$^+$ and anions H$^-$ through I$^-$, we performed numerical Hartree–Fock calculations using a modified and enhanced version of the MCHF72 program [29]. The experimental ground states [30, 31] (see Ref. [32] for an explicit tabulation) were considered for all species except for two anions. For Sc$^-$and Pd$^-$, the experimental ground states were reported [31] to be [Ar]$4s^2 3d4p$, ^{1}D and [Kr]$5s4d^{10}$, ^{2}S, respectively, but we could not obtain meaningful solutions for these states in numerical (and Roothaan–) Hartree–Fock calculations. Thus the second-lowest states, [Ar]$4s^2 3d^{\,2}$, ^{3}F for Sc$^-$ and [Kr]$5s^2 4d^9$, ^{2}D for Pd$^-$, were examined instead.

In our numerical Hartree–Fock calculations, the radial mesh in position space was generated by the formula $r_i = Z^{-1}\exp[x_{\min} + (i-1)h]$ ($i = 1, 2, \ldots, N_p$), where the parameters were chosen to be $x_{\min} = -16$, $h = 1/40$, and $N_p = 2^{10} = 1024$. These values of the discretization parameters were based on our previous study [10] of neutral atoms except that h was halved and N_p was doubled, because anionic species include very diffuse position-space orbitals compared to neutral and cationic species. The radial convergence condition was 1×10^{-10} for any radial point r_i of any radial function $R_{nl}(r_i)$ of occupied atomic orbitals $\psi_{nlm}(\mathbf{r}) = R_{nl}(r)Y_{lm}(\Omega_r)$, where $Y_{lm}(\Omega_r)$ is a spherical harmonic. Following the formulae given in Ref. [2], appropriate integrations of the radial functions $R_{nl}(r)$ gave the small-p expansion coefficients (Eq. 2a), while the values of $R_{nl}(r)/r^l$ at $r = 0$ gave the leading coefficient of the large-p expansion (Eq. 4a) of the momentum density $\Pi(p)$. Since atomic momentals (momentum-space orbitals) $\phi_{nlm}(\mathbf{p})$ are given [7] by

$$\begin{aligned}\phi_{nlm}(\mathbf{p}) &= (2\pi)^{-3/2}\int \mathrm{d}\mathbf{r}\, \exp(-i\mathbf{p}\cdot\mathbf{r})\,\psi_{nlm}(\mathbf{r}) \\ &= P_{nl}(p)Y_{lm}(\Omega_p) \ ,\end{aligned} \tag{8a}$$

$$P_{nl}(p) = (-i)^l (2/\pi)^{1/2}\int_0^\infty \mathrm{d}r\, r^2 j_l(pr)R_{nl}(r) \ , \tag{8b}$$

where $j_l(x)$ is the lth order spherical Bessel function of the first kind, the radial momentals $P_{nl}(p_i)$ were obtained by numerical Hankel transformation (Eq. 8b) of $R_{nl}(r_i)$, using the algorithm of Talman [33]. The radial mesh in momentum space was generated by the formula $p_i = Z\exp[y_{\min} + (i-1)h]$ ($i = 1, 2, \ldots, N_p$), where we adopted $y_{\min} = -17$. The normalization error of the Hankel transformation was less than 1×10^{-12} for all orbitals. The momentum moments $\langle p^k\rangle$ were computed by numerical integration.

3 Asymptotic expansion coefficients of momentum densities

The expansion coefficients of $\Pi(p)$ for small and large momenta, defined by Eqs. (2a) and (4a), are summarized

Table 1. Hartree–Fock momentum density expansion coefficients for the ground-state cations He^+ ($Z=2$) to Cs^+ ($Z=55$). Normalization for the momentum density is $\langle 1\rangle = N = Z-1$. $A(\pm n)$ means $A \times 10^{\pm n}$

Cation	$\Pi(0)$	$\Pi^{ii}(0)/2!$	$\Pi^{iv}(0)/4!$	b_8
2 He^+	1.0132 (−1)	−1.0132 (−1)	6.3326 (−2)	8.1057 (−1)
3 Li^+	9.7700 (−2)	−6.3348 (−2)	2.6259 (−2)	1.2895
4 Be^+	1.6355	−8.0275	2.2206 (+1)	1.3956
5 B^+	1.6899	−5.6318	1.0706 (+1)	1.4796
6 C^+	9.6336 (−1)	−1.8251	1.9049	1.5143
7 N^+	6.0395 (−1)	−6.5094 (−1)	2.5465 (−1)	1.5390
8 O^+	4.0457 (−1)	−2.3201 (−1)	−7.2471 (−2)	1.5574
9 F^+	2.8184 (−1)	−2.6220 (−2)	−1.9979 (−1)	1.5725
10 Ne^+	2.0475 (−1)	4.4848 (−2)	−1.8202 (−1)	1.5844
11 Na^+	1.5369 (−1)	6.4825 (−2)	−1.3926 (−1)	1.5941
12 Mg^+	2.8393	−1.9173 (+1)	7.2271 (+1)	1.6106
13 Al^+	3.5827	−1.8733 (+1)	5.4358 (+1)	1.6271
14 Si^+	2.2841	−5.8078	3.8844	1.6396
15 P^+	1.5719	−1.7627	−3.3822	1.6507
16 S^+	1.1386	−3.3222 (−1)	−3.6108	1.6605
17 Cl^+	8.5287 (−1)	4.5790 (−1)	−3.8251	1.6695
18 Ar^+	6.5840 (−1)	6.8022 (−1)	−3.0451	1.6775
19 K^+	5.2050 (−1)	6.9024 (−1)	−2.2359	1.6847
20 Ca^+	5.7458	−5.8199 (+1)	3.2933 (+2)	1.6930
21 Sc^+	4.7602	−4.2966 (+1)	2.1793 (+2)	1.6996
22 Ti^+	4.1159	−3.4046 (+1)	1.5861 (+2)	1.7056
23 V^+	2.2208 (−1)	1.0962 (−1)	1.4867	1.7101
24 Cr^+	1.8883 (−1)	7.8517 (−2)	1.0255	1.7151
25 Mn^+	2.9124	−1.9608 (+1)	7.4707 (+1)	1.7208
26 Fe^+	2.6959	−1.7369 (+1)	6.3350 (+1)	1.7251
27 Co^+	1.2124 (−1)	3.1297 (−2)	6.8947 (−1)	1.7282
28 Ni^+	1.0637 (−1)	2.3918 (−2)	5.7638 (−1)	1.7320
29 Cu^+	9.4004 (−2)	1.8581 (−2)	4.6982 (−1)	1.7355
30 Zn^+	2.1206	−1.1935 (+1)	3.8028 (+1)	1.7395
31 Ga^+	3.1872	−1.5471 (+1)	4.1866 (+1)	1.7437
32 Ge^+	2.3130	−5.3910	4.4391 (−1)	1.7472
33 As^+	1.7629	−1.5812	−7.1291	1.7505
34 Se^+	1.3891	−2.1665 (−3)	−7.4518	1.7537
35 Br^+	1.1190	1.1035	−8.3238	1.7567
36 Kr^+	9.2001 (−1)	1.4825	−7.2642	1.7596
37 Rb^+	7.6866 (−1)	1.5403	−5.8432	1.7624
38 Sr^+	7.4296	−8.6898 (+1)	5.7209 (+2)	1.7654
39 Y^+	1.0225 (+1)	−1.0143 (+2)	5.4548 (+2)	1.7684
40 Zr^+	5.0900	−4.6919 (+1)	2.4812 (+2)	1.7707
41 Nb^+	3.7266 (−1)	3.0394 (−1)	4.0360	1.7728
42 Mo^+	3.2514 (−1)	2.2696 (−1)	2.7107	1.7752
43 Tc^+	3.5982	−2.6931 (+1)	1.1604 (+2)	1.7777
44 Ru^+	2.5263 (−1)	1.3253 (−1)	1.9171	1.7796
45 Rh^+	2.2531 (−1)	1.0398 (−1)	1.5369	1.7816
46 Pd^+	2.0216 (−1)	8.2681 (−2)	1.2324	1.7836
47 Ag^+	1.8244 (−1)	6.6563 (−2)	9.7234 (−1)	1.7855
48 Cd^+	2.8709	−1.9121 (+1)	7.2399 (+1)	1.7876
49 In^+	4.4403	−2.6349 (+1)	8.6444 (+1)	1.7898
50 Sn^+	3.3660	−1.0318 (+1)	5.9331	1.7917
51 Sb^+	2.6598	−3.5644	−1.3058 (+1)	1.7935
52 Te^+	2.1620	−4.4623 (−1)	−1.6198 (+1)	1.7953
53 I^+	1.7920	1.8658	−1.9866 (+1)	1.7970
54 Xe^+	1.5109	2.8324	−1.8544 (+1)	1.7987
55 Cs^+	1.2913	3.1409	−1.5800 (+1)	1.8003

in Table 1 for the cations and in Table 2 for the anions. In the small-p expansion, we observed for neutral atoms with $N \leq 54$ [3, 10] that the leading coefficients $\Pi(0)$ generally decrease from the group 1 to the group 18 atom within a period, with some exceptions for transition-metal atoms due to irregularities in the occupation numbers of the outermost s and d subshells. An analogous trend is found for the $\Pi(0)$ values of the cations and anions, and yet we have a general inequality $\Pi^+(0) < \Pi^0(0) < \Pi^-(0)$ for all the isoelectronic cases, where the superscripts +, 0, and – refer to the cationic, neutral, and anionic properties, respectively. Previously [34], the Hartree–Fock momentum densities $\Pi(p)$ of neutral and singly charged atoms were shown to be separated into three distinct categories according to their modalities:

Table 2. Hartree–Fock momentum density expansion coefficients for the ground-state anions H$^-$ ($Z = 1$) to I$^-$ ($Z = 53$). Normalization for the momentum density is $\langle 1 \rangle = N = Z + 1$. $A(\pm n)$ means $A \times 10^{\pm n}$

Anion	$\Pi(0)$	$\Pi^{ii}(0)/2!$	$\Pi^{iv}(0)/4!$	b_8
1 H$^-$	1.2417 (+1)	−2.8000 (+2)	4.6138 (+3)	7.8735 (−1)
3 Li$^-$	1.0086 (+2)	−7.6413 (+3)	4.0921 (+5)	1.3026
5 B$^-$	3.7572	1.4849 (+2)	−7.1127 (+3)	1.4591
6 C$^-$	1.8848	1.8273 (+1)	−3.6589 (+2)	1.4963
7 N$^-$	1.0329	1.3212 (+1)	−1.8405 (+2)	1.5250
8 O$^-$	6.3572 (−1)	7.1849	−6.9713 (+1)	1.5460
9 F$^-$	4.2138 (−1)	3.8776	−2.6737 (+1)	1.5621
11 Na$^-$	1.1875 (+2)	−9.8662 (+3)	5.7703 (+5)	1.5951
13 Al$^-$	6.7901	5.0309 (+2)	−3.1549 (+4)	1.6255
14 Si$^-$	3.9222	6.7742 (+1)	−1.7162 (+3)	1.6379
15 P$^-$	2.4628	4.5499 (+1)	−8.2619 (+2)	1.6491
16 S$^-$	1.6804	2.5514 (+1)	−3.2692 (+2)	1.6590
17 Cl$^-$	1.2097	1.4531 (+1)	−1.3445 (+2)	1.6679
19 K$^-$	1.9249 (+2)	−2.1140 (+4)	1.6146 (+6)	1.6850
21 Sc$^-$	9.7699 (+1)	−6.8844 (+3)	3.3812 (+5)	1.6991
22 Ti$^-$	9.4883 (+1)	−6.6704 (+3)	3.2847 (+5)	1.7051
23 V$^-$	8.9148 (+1)	−6.0750 (+3)	2.9080 (+5)	1.7106
24 Cr$^-$	8.5138 (+1)	−5.6760 (+3)	2.6643 (+5)	1.7156
25 Mn$^-$	7.5137 (+1)	−4.6366 (+3)	2.0177 (+5)	1.7203
26 Fe$^-$	6.8685 (+1)	−4.0170 (+3)	1.6593 (+5)	1.7246
27 Co$^-$	6.3485 (+1)	−3.5439 (+3)	1.3994 (+5)	1.7287
28 Ni$^-$	5.9157 (+1)	−3.1683 (+3)	1.2019 (+5)	1.7324
29 Cu$^-$	5.6031 (+1)	−2.9103 (+3)	1.0722 (+5)	1.7359
31 Ga$^-$	5.7089	6.2793 (+2)	−4.1969 (+4)	1.7434
32 Ge$^-$	3.8206	8.1830 (+1)	−2.0642 (+3)	1.7469
33 As$^-$	2.6825	5.8158 (+1)	−1.0971 (+3)	1.7502
34 Se$^-$	2.0018	3.5499 (+1)	−4.8646 (+2)	1.7534
35 Br$^-$	1.5532	2.2057 (+1)	−2.2419 (+2)	1.7564
37 Rb$^-$	2.2411 (+2)	−2.6862 (+4)	2.2295 (+6)	1.7625
39 Y$^-$	3.1260 (+1)	1.1998 (+4)	−4.2690 (+6)	1.7682
40 Zr$^-$	8.9269 (+1)	−5.8371 (+3)	2.6477 (+5)	1.7706
41 Nb$^-$	8.6379 (+1)	−5.6111 (+3)	2.5401 (+5)	1.7730
42 Mo$^-$	8.5141 (+1)	−5.5460 (+3)	2.5266 (+5)	1.7753
43 Tc$^-$	7.6968 (+1)	−4.7129 (+3)	2.0213 (+5)	1.7776
44 Ru$^-$	7.2527 (+1)	−4.2973 (+3)	1.7868 (+5)	1.7797
45 Rh$^-$	6.9289 (+1)	−4.0084 (+3)	1.6301 (+5)	1.7818
46 Pd$^-$	6.6810 (+1)	−3.7953 (+3)	1.5181 (+5)	1.7838
47 Ag$^-$	6.5388 (+1)	−3.6834 (+3)	1.4633 (+5)	1.7857
49 In$^-$	8.0820	5.1132 (+2)	−3.1546 (+4)	1.7897
50 Sn$^-$	5.5658	9.2168 (+1)	−2.6039 (+3)	1.7916
51 Sb$^-$	4.0496	7.6341 (+1)	−1.6141 (+3)	1.7934
52 Te$^-$	3.1154	5.1854 (+1)	−8.1497 (+2)	1.7952
53 I$^-$	2.4828	3.5065 (+1)	−4.1805 (+2)	1.7969

Type 1. Unimodal $\Pi(p)$ with a maximum at $p = 0$.

Type 2. Unimodal $\Pi(p)$ with a local minimum at $p = 0$ and a maximum at $p_{\max} > 0$.

Type 3. Bimodal $\Pi(p)$ with a primary maximum at $p = 0$, a secondary maximum at $p_{\max} > 0$, and a local minimum at $p_{\min}$ with $0 < p_{\min} < p_{\max}$.

Then, another noticeable point is that the $\Pi(0)$ values are exceptionally large for the anions with type 1 and 3 momentum densities. The largest is 224.11 for Rb$^-$, which should be compared with 23.95 for Sr and 10.23 for Y$^+$ with the same [Kr]$5s^2$ electronic configuration.

As in the neutral atoms [3, 34], the sign of $\Pi^{ii}(0)$ reflects the modality of the momentum density. The coefficient is negative for a type 1 or 3 momentum density with a primary maximum at $p = 0$, while it is positive for a type 2 momentum density with a local minimum at $p = 0$. In general, we find the inequality $|\Pi^{ii+}(0)| < |\Pi^{ii0}(0)| < |\Pi^{ii-}(0)|$ with two exceptions for the $N = 14$ (P$^+$, Si, Al$^-$) and $N = 50$ (Sb$^+$, Sn, In$^-$) series where $|\Pi^{ii0}(0)| < |\Pi^{ii+}(0)| < |\Pi^{ii-}(0)|$. Anions that have very large values of $\Pi(0)$ also have exceptionally large values of $|\Pi^{ii}(0)|$ and $|\Pi^{iv}(0)|$; however, there is no one-to-one correspondence between the sign of $\Pi^{iv}(0)$ and the modality of $\Pi(p)$, although we observe $\mathrm{sign}[\Pi^{ii}(0)] = -\mathrm{sign}[\Pi^{iv}(0)]$ for 35 cations and all 43 anions. The leading coefficients b_8 for the large-p expansion are not very different among isoelectronic species and increase smoothly with increasing N. Generally, the relation $b_8^- < b_8^0 \leq b_8^+$ is valid without exception, where the equality holds only for $N = 1$ (H and He$^+$).

For the Hartree–Fock ground states of the ions, Thakkar et al. [3] reported the expansion coefficients of $\Pi(p)$, based on the approximate wave functions of Clementi and Roetti [22] for Li$^+$ to Xe$^+$ and Li$^-$ to I$^-$ and of McLean and McLean [23] for Cs$^+$ to Ra$^+$. We

Table 3. Hartree–Fock momentum moments for the ground-state cations He$^+$ ($Z=2$) to Cs$^+$ ($Z=55$). Normalization is $\langle 1 \rangle = N = Z–1$. $A(\pm n)$ means $A \times 10^{\pm n}$

Cation	$\langle p^{-2} \rangle$	$\langle p^{-1} \rangle$	$\langle p \rangle$	$\langle p^2 \rangle$	$\langle p^3 \rangle$	$\langle p^4 \rangle$
2 He$^+$	1.2500	8.4883 (−1)	1.6977	4.0000	1.3581 (+1)	8.0000 (+1)
3 Li$^+$	1.5162	1.3111	4.4972	1.4473 (+1)	6.9878 (+1)	6.1482 (+2)
4 Be$^+$	9.0194	3.1545	6.9503	2.8555 (+1)	1.8319 (+2)	2.1353 (+3)
5 B$^+$	1.1093 (+1)	4.2718	9.8229	4.8475 (+1)	3.8640 (+2)	5.5942 (+3)
6 C$^+$	8.4555	4.3382	1.3511 (+1)	7.4584 (+1)	6.9530 (+2)	1.1966 (+4)
7 N$^+$	6.7923	4.3845	1.7786 (+1)	1.0778 (+2)	1.1414 (+3)	2.2685 (+4)
8 O$^+$	5.6563	4.4194	2.2647 (+1)	1.4875 (+2)	1.7533 (+3)	3.9406 (+4)
9 F$^+$	4.8872	4.4858	2.7969 (+1)	1.9766 (+2)	2.5604 (+3)	6.4098 (+4)
10 Ne$^+$	4.2976	4.5340	3.3876 (+1)	2.5564 (+2)	3.5945 (+3)	9.8972 (+4)
11 Na$^+$	3.8304	4.5698	4.0368 (+1)	3.2335 (+2)	4.8890 (+3)	1.4655 (+5)
12 Mg$^+$	1.4638 (+1)	6.5847	4.6127 (+1)	3.9874 (+2)	6.5001 (+3)	2.1083 (+5)
13 Al$^+$	1.9620 (+1)	7.9844	5.2144 (+1)	4.8335 (+2)	8.4519 (+3)	2.9483 (+5)
14 Si$^+$	1.6682 (+1)	8.2496	5.8614 (+1)	5.7715 (+2)	1.0760 (+4)	4.0140 (+5)
15 P$^+$	1.4525 (+1)	8.4177	6.5432 (+1)	6.8070 (+2)	1.3469 (+4)	5.3480 (+5)
16 S$^+$	1.2864 (+1)	8.5324	7.2597 (+1)	7.9435 (+2)	1.6614 (+4)	6.9924 (+5)
17 Cl$^+$	1.1685 (+1)	8.6744	8.0022 (+1)	9.1810 (+2)	2.0231 (+4)	8.9931 (+5)
18 Ar$^+$	1.0683 (+1)	8.7749	8.7792 (+1)	1.0525 (+3)	2.4356 (+4)	1.1399 (+6)
19 K$^+$	9.8245	8.8476	9.5905 (+1)	1.1980 (+3)	2.9029 (+4)	1.4261 (+6)
20 Ca$^+$	2.6081 (+1)	1.1160 (+1)	1.0360 (+2)	1.3531 (+3)	3.4301 (+4)	1.7663 (+6)
21 Sc$^+$	2.3305 (+1)	1.0989 (+1)	1.1239 (+2)	1.5191 (+3)	4.0145 (+4)	2.1613 (+6)
22 Ti$^+$	2.1271 (+1)	1.0837 (+1)	1.2163 (+2)	1.6964 (+3)	4.6625 (+4)	2.6192 (+6)
23 V$^+$	6.9344	8.7228	1.3211 (+2)	1.8853 (+3)	5.3725 (+4)	3.1419 (+6)
24 Cr$^+$	6.4136	8.6551	1.4220 (+2)	2.0863 (+3)	6.1582 (+4)	3.7442 (+6)
25 Mn$^+$	1.7037 (+1)	1.0475 (+1)	1.5171 (+2)	2.2993 (+3)	7.0255 (+4)	4.4357 (+6)
26 Fe$^+$	1.6185 (+1)	1.0418 (+1)	1.6239 (+2)	2.5244 (+3)	7.9653 (+4)	5.2125 (+6)
27 Co$^+$	5.3390	8.5717	1.7442 (+2)	2.7623 (+3)	8.9795 (+4)	6.0791 (+6)
28 Ni$^+$	5.0501	8.5415	1.8592 (+2)	3.0132 (+3)	1.0087 (+5)	7.0586 (+6)
29 Cu$^+$	4.7837	8.5076	1.9782 (+2)	3.2775 (+3)	1.1283 (+5)	8.1523 (+6)
30 Zn$^+$	1.3686 (+1)	1.0214 (+1)	2.0901 (+2)	3.5551 (+3)	1.2583 (+5)	9.3818 (+6)
31 Ga$^+$	1.9530 (+1)	1.1604 (+1)	2.2033 (+2)	3.8461 (+3)	1.3985 (+5)	1.0747 (+7)
32 Ge$^+$	1.8189 (+1)	1.2011 (+1)	2.3197 (+2)	4.1502 (+3)	1.5488 (+5)	1.2244 (+7)
33 As$^+$	1.6993 (+1)	1.2304 (+1)	2.4383 (+2)	4.4678 (+3)	1.7100 (+5)	1.3895 (+7)
34 Se$^+$	1.5940 (+1)	1.2527 (+1)	2.5591 (+2)	4.7991 (+3)	1.8825 (+5)	1.5709 (+7)
35 Br$^+$	1.5195 (+1)	1.2772 (+1)	2.6815 (+2)	5.1441 (+3)	2.0667 (+5)	1.7699 (+7)
36 Kr$^+$	1.4478 (+1)	1.2962 (+1)	2.8062 (+2)	5.5031 (+3)	2.2630 (+5)	1.9873 (+7)
37 Rb$^+$	1.3801 (+1)	1.3112 (+1)	2.9332 (+2)	5.8764 (+3)	2.4719 (+5)	2.2244 (+7)
38 Sr$^+$	3.2854 (+1)	1.5584 (+1)	3.0565 (+2)	6.2627 (+3)	2.6939 (+5)	2.4829 (+7)
39 Y$^+$	4.3648 (+1)	1.7430 (+1)	3.1812 (+2)	6.6629 (+3)	2.9294 (+5)	2.7635 (+7)
40 Zr$^+$	2.6848 (+1)	1.5336 (+1)	3.3216 (+2)	7.0776 (+3)	3.1769 (+5)	3.0658 (+7)
41 Nb$^+$	1.0867 (+1)	1.3246 (+1)	3.4650 (+2)	7.5068 (+3)	3.4384 (+5)	3.3924 (+7)
42 Mo$^+$	1.0231 (+1)	1.3196 (+1)	3.6053 (+2)	7.9507 (+3)	3.7150 (+5)	3.7454 (+7)
43 Tc$^+$	2.1946 (+1)	1.5033 (+1)	3.7407 (+2)	8.4092 (+3)	4.0073 (+5)	4.1264 (+7)
44 Ru$^+$	9.2776	1.3165 (+1)	3.8923 (+2)	8.8826 (+3)	4.3130 (+5)	4.5337 (+7)
45 Rh$^+$	8.8501	1.3136 (+1)	4.0398 (+2)	9.3713 (+3)	4.6353 (+5)	4.9717 (+7)
46 Pd$^+$	8.4573	1.3106 (+1)	4.1900 (+2)	9.8754 (+3)	4.9737 (+5)	5.4409 (+7)
47 Ag$^+$	8.0887	1.3069 (+1)	4.3429 (+2)	1.0395 (+4)	5.3285 (+5)	5.9427 (+7)
48 Cd$^+$	1.8687 (+1)	1.4886 (+1)	4.4893 (+2)	1.0930 (+4)	5.7016 (+5)	6.4803 (+7)
49 In$^+$	2.6068 (+1)	1.6393 (+1)	4.6368 (+2)	1.1480 (+4)	6.0924 (+5)	7.0540 (+7)
50 Sn$^+$	2.4806 (+1)	1.6860 (+1)	4.7871 (+2)	1.2045 (+4)	6.5009 (+5)	7.6641 (+7)
51 Sb$^+$	2.3622 (+1)	1.7207 (+1)	4.9391 (+2)	1.2626 (+4)	6.9278 (+5)	8.3133 (+7)
52 Te$^+$	2.2539 (+1)	1.7480 (+1)	5.0929 (+2)	1.3223 (+4)	7.3738 (+5)	9.0033 (+7)
53 I$^+$	2.1796 (+1)	1.7779 (+1)	5.2478 (+2)	1.3835 (+4)	7.8390 (+5)	9.7358 (+7)
54 Xe$^+$	2.1045 (+1)	1.8018 (+1)	5.4045 (+2)	1.4463 (+4)	8.3242 (+5)	1.0512 (+8)
55 Cs$^+$	2.0311 (+1)	1.8213 (+1)	5.5631 (+2)	1.5108 (+4)	8.8296 (+5)	1.1335 (+8)

have compared their values with the present ones for 51 cations and 38 anions, excluding He$^+$, V$^+$, and Fe$^+$ from our 54 cations and H$^-$, Ga$^-$, Y$^-$, Tc$^-$, and Ru$^-$ from our 43 anions since corresponding coefficients were either not reported at all or were reported for a different state in Ref. [3]. For the 51 cations, the average (and the largest) errors in the Clementi–Roetti coefficients $\Pi(0)$, $\Pi^{ii}(0)/2!$, $\Pi^{iv}(0)/4!$, and b_8, relative to the present numerical Hartree–Fock values, are 0.8% (7.4% for Y$^+$), 192.9% (9538.1% for Se$^+$), 58.8% (2328.0% for Ge$^+$), and 0.3% (1.3% for Be$^+$), respectively. The Clementi–Roetti values of $\Pi(0)$ and b_8 may be acceptable, but those for the other two coefficients are certainly not. Unlike the case of the neutral Si atom [10], all four Clementi–Roetti coefficients for the 97 ions have the correct sign. For the 38 anions, the corresponding errors

Table 4. Hartree–Fock momentum moments for the ground-state anions H$^-$ ($Z = 1$) to I$^-$ ($Z = 53$). Normalization is $\langle 1 \rangle = N = Z + 1$. $A(\pm n)$ means $A \times 10^{\pm n}$

Anion	$\langle p^{-2} \rangle$	$\langle p^{-1} \rangle$	$\langle p \rangle$	$\langle p^2 \rangle$	$\langle p^3 \rangle$	$\langle p^4 \rangle$
1 H$^-$	3.5317 (+1)	6.0314	1.0973	9.7586 (−1)	1.4603	4.3477
3 Li$^-$	1.5248 (+2)	1.4233 (+1)	5.0188	1.4856 (+1)	7.0929 (+1)	6.2652 (+2)
5 B$^-$	2.8056 (+1)	8.8691	1.1057 (+1)	4.9038 (+1)	3.8171 (+2)	5.5131 (+3)
6 C$^-$	1.7973 (+1)	7.8532	1.5020 (+1)	7.5418 (+1)	6.8797 (+2)	1.1815 (+4)
7 N$^-$	1.3734 (+1)	7.4790	1.9410 (+1)	1.0864 (+2)	1.1315 (+3)	2.2460 (+4)
8 O$^-$	1.0870 (+1)	7.1557	2.4394 (+1)	1.4958 (+2)	1.7399 (+3)	3.9085 (+4)
9 F$^-$	8.8649	6.8890	2.9965 (+1)	1.9892 (+2)	2.5433 (+3)	6.3624 (+4)
11 Na$^-$	1.7282 (+2)	1.8272 (+1)	4.0840 (+1)	3.2371 (+2)	4.8927 (+3)	1.4684 (+5)
13 Al$^-$	4.6796 (+1)	1.4063 (+1)	5.3030 (+1)	4.8376 (+2)	8.4457 (+3)	2.9454 (+5)
14 Si$^-$	3.2688 (+1)	1.2989 (+1)	5.9697 (+1)	5.7778 (+2)	1.0752 (+4)	4.0098 (+5)
15 P$^-$	2.6879 (+1)	1.2669 (+1)	6.6593 (+1)	6.8140 (+2)	1.3460 (+4)	5.3428 (+5)
16 S$^-$	2.2520 (+1)	1.2347 (+1)	7.3840 (+1)	7.9508 (+2)	1.6603 (+4)	6.9860 (+5)
17 Cl$^-$	1.9247 (+1)	1.2060 (+1)	8.1433 (+1)	9.1915 (+2)	2.0219 (+4)	8.9849 (+5)
19 K$^-$	2.4489 (+2)	2.5053 (+1)	9.6312 (+1)	1.1983 (+3)	2.9034 (+4)	1.4545 (+6)
21 Sc$^-$	1.5768 (+2)	2.1876 (+1)	1.1350 (+2)	1.5194 (+3)	4.0120 (+4)	2.1878 (+6)
22 Ti$^-$	1.5338 (+2)	2.1581 (+1)	1.2283 (+2)	1.6967 (+3)	4.6594 (+4)	2.6550 (+6)
23 V$^-$	1.4649 (+2)	2.1209 (+1)	1.3253 (+2)	1.8857 (+3)	5.3743 (+4)	3.1925 (+6)
24 Cr$^-$	1.4147 (+2)	2.0915 (+1)	1.4263 (+2)	2.0867 (+3)	6.1601 (+4)	3.8091 (+6)
25 Mn$^-$	1.3011 (+2)	2.0383 (+1)	1.5299 (+2)	2.2995 (+3)	7.0214 (+4)	4.5060 (+6)
26 Fe$^-$	1.2237 (+2)	1.9989 (+1)	1.6375 (+2)	2.5247 (+3)	7.9608 (+4)	5.2972 (+6)
27 Co$^-$	1.1593 (+2)	1.9647 (+1)	1.7489 (+2)	2.7627 (+3)	8.9824 (+4)	6.1895 (+6)
28 Ni$^-$	1.1041 (+2)	1.9344 (+1)	1.8640 (+2)	3.0136 (+3)	1.0090 (+5)	7.1913 (+6)
29 Cu$^-$	1.0626 (+2)	1.9100 (+1)	1.9831 (+2)	3.2779 (+3)	1.1287 (+5)	8.3129 (+6)
31 Ga$^-$	4.5980 (+1)	1.7635 (+1)	2.2120 (+2)	3.8465 (+3)	1.3984 (+5)	1.0756 (+7)
32 Ge$^-$	3.4392 (+1)	1.6818 (+1)	2.3300 (+2)	4.1508 (+3)	1.5487 (+5)	1.2250 (+7)
33 As$^-$	3.0314 (+1)	1.6747 (+1)	2.4491 (+2)	4.4684 (+3)	1.7099 (+5)	1.3899 (+7)
34 Se$^-$	2.6891 (+1)	1.6613 (+1)	2.5705 (+2)	4.7998 (+3)	1.8824 (+5)	1.5712 (+7)
35 Br$^-$	2.4133 (+1)	1.6473 (+1)	2.6942 (+2)	5.1451 (+3)	2.0666 (+5)	1.7701 (+7)
37 Rb$^-$	2.7445 (+2)	3.0183 (+1)	2.9370 (+2)	5.8767 (+3)	2.4720 (+5)	2.2291 (+7)
39 Y$^-$	1.1819 (+2)	2.6127 (+1)	3.1925 (+2)	6.6634 (+3)	2.9288 (+5)	2.7636 (+7)
40 Zr$^-$	1.5235 (+2)	2.5912 (+1)	3.3316 (+2)	7.0780 (+3)	3.1766 (+5)	3.0685 (+7)
41 Nb$^-$	1.4804 (+2)	2.5661 (+1)	3.4692 (+2)	7.5072 (+3)	3.4388 (+5)	3.3964 (+7)
42 Mo$^-$	1.4569 (+2)	2.5494 (+1)	3.6097 (+2)	7.9511 (+3)	3.7153 (+5)	3.7500 (+7)
43 Tc$^-$	1.3623 (+2)	2.5067 (+1)	3.7518 (+2)	8.4095 (+3)	4.0068 (+5)	4.1303 (+7)
44 Ru$^-$	1.3067 (+2)	2.4788 (+1)	3.8969 (+2)	8.8831 (+3)	4.3134 (+5)	4.5392 (+7)
45 Rh$^-$	1.2643 (+2)	2.4563 (+1)	4.0445 (+2)	9.3718 (+3)	4.6357 (+5)	4.9778 (+7)
46 Pd$^-$	1.2306 (+2)	2.4375 (+1)	4.1948 (+2)	9.8758 (+3)	4.9741 (+5)	5.4478 (+7)
47 Ag$^-$	1.2092 (+2)	2.4239 (+1)	4.3478 (+2)	1.0395 (+4)	5.3290 (+5)	5.9504 (+7)
49 In$^-$	5.5138 (+1)	2.2717 (+1)	4.6450 (+2)	1.1480 (+4)	6.0923 (+5)	7.0542 (+7)
50 Sn$^-$	4.4125 (+1)	2.2093 (+1)	4.7966 (+2)	1.2046 (+4)	6.5007 (+5)	7.6641 (+7)
51 Sb$^-$	3.9915 (+1)	2.2113 (+1)	4.9489 (+2)	1.2627 (+4)	6.9277 (+5)	8.3132 (+7)
52 Te$^-$	3.6270 (+1)	2.2050 (+1)	5.1031 (+2)	1.3224 (+4)	7.3736 (+5)	9.0031 (+7)
53 I$^-$	3.3242 (+1)	2.1965 (+1)	5.2591 (+2)	1.3836 (+4)	7.8389 (+5)	9.7355 (+7)

are 12.0% (−52.7% for Rb$^-$), 31.7% (−81.1% for Rb$^-$), 51.0% (−94.2% for Rb$^-$), and 0.3% (1.3% for Li$^-$). Except for Ge$^+$and Se$^+$, where large errors in small values produce enormous percentage errors, the errors are larger in general for the anions than for the cations. The above comparison again clarifies inaccuracies [24–26, 28] of the Clementi–Roetti wave functions, particularly for anions [26].

4 Moments of momentum densities

The finite moments $\langle p^k \rangle$ ($-2 \le k \le +4$) of the momentum density $\Pi(p)$, defined by Eq. (5), are listed in Table 3 for the cations and in Table 4 for the anions. As seen for the neutral atoms [10, 35], the moments $\langle p^k \rangle$ with positive k are largely governed by inner electrons and also increase smoothly with increasing N for charged atoms. For positive values of k, we generally have $\langle p^k \rangle^- < \langle p^k \rangle^0 < \langle p^k \rangle^+$ for isoelectronic species without exception, reflecting the increasing compaction of the core as the nuclear charge is increased in an isoelectronic series. On the other hand, the moments $\langle p^k \rangle$ with negative k show strong periodic behavior reflecting the difference in valence electronic configurations and properties of outer orbitals. As far as species with $N \le 54$ are concerned, the inequality $\langle p^k \rangle^+ < \langle p^k \rangle^0 < \langle p^k \rangle^-$ is true for negative k. In particular, the anions with type 1 momentum densities have large $\langle p^{-1} \rangle$ and $\langle p^{-2} \rangle$ values as anticipated from their $\Pi(0)$ values discussed previously.

Using the Clementi–Roetti wave functions [22], Gadre et al. [17] computed momentum moments of singly charged ions. They examined the experimental ground states for 52 cations (excluding He$^+$ and Cs$^+$ from the present 54 cations) and 39 anions (excluding

H$^-$, Ga$^-$, Y$^-$, and Ru$^-$ from the present 43 anions). For the 52 cations, the average errors in the Clementi–Roetti moments $\langle p^k \rangle$, relative to the present numerical Hartree–Fock values, are 0.30, 0.05, 0.00, 0.00, 0.01, and 0.09%, respectively, for $k = -2, -1, 1, 2, 3$, and 4. In contrast to the examination of the expansion coefficients described earlier, the momentum moments from the approximate Clementi–Roetti functions are found to have relatively good accuracy for the cations, partly due to the cancellation of local errors upon integration. For the 39 anions, however, the errors in the Clementi–Roetti $\langle p^k \rangle$ values are larger. The average (and the largest) errors are 5.72% (-32.41% at Rb$^-$) for $\langle p^{-2} \rangle$, 1.15% (-8.70% at Rb$^-$) for $\langle p^{-1} \rangle$, 0.02% (-0.49% at Tc$^-$) for $\langle p \rangle$, 0.02% (-0.64% at Tc$^-$) for $\langle p^2 \rangle$, 0.02% (-0.37% at Tc$^-$) for $\langle p^3 \rangle$, and 0.55% (-1.94% at K$^-$) for $\langle p^4 \rangle$. The larger errors for the moments $\langle p^{-2} \rangle$ and $\langle p^{-1} \rangle$ imply that the Clementi–Roetti functions for anions are particularly poor in the description of their very diffuse valence or outer orbitals, as pointed out in Ref. [26], since momentum and position spaces emphasize reciprocal regions of space.

5 Summary

The first three coefficients of the MacLaurin expansion, the leading coefficient of the large-p asymptotic expansion, and the finite moments $\langle p^k \rangle$ of $\Pi(p)$ were computed for a series of 54 singly charged atomic cations from He$^+$ to Cs$^+$ and 43 anions from H$^-$ to I$^-$ in their experimental ground state, using the numerical Hartree–Fock method. Nontrivial errors were pointed out for these properties reported previously based on the approximate basis-set-expansion wave functions of Clementi and Roetti. The present results were compared with the corresponding ones for neutral atoms, and the Z dependence of the expansion coefficients and moments was discussed for isoelectronic species.

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