Analytic functions for atomic momentum-density distributions and Compton profiles of K and L shells

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An analytical expression involving three parameters was proposed for atomic momentum-density distributions of K and L shells. This expression was based on the superposition of hydrogenic closed-shell momentum densities. Parameters in the expression were determined by requiring four of its moments to be equal to the corresponding Hartree-Fock results. An analytical function for the Compton profiles was then derived using the impulse approximation. Excellent agreement was found between the present results and detailed theoretical computations.

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I. INTRODUCTION

The atomic electron-density distribution in momentum space plays an important role in many applications. For instance, this distribution is directly related to Compton profiles, which represent the Doppler broadening of Compton lines due to moving electrons [1]. Moreover, this distribution is needed for the calculation of stopping cross sections, shell corrections, and ionization cross sections by the binary-encounter theory [2,3]. Thus, a study of the momentum-density distribution is important.

In all these applications, a simple analytical function for atomic momentum densities for each shell is desired. This function will help the manipulation of such densities, usually calculated by the Hartree-Fock (HF) approach with data presented in tabulated form, in a very simple way. Although an analytical expression for momentum-space wave functions in the configurational Slater-type orbitals was reported [4] and hence an atomic momentum-density distribution could be derived, this expression involved too many terms and parameters to be of useful applications.

In this work, we propose a simple analytical form involving three parameters for atomic momentum-density distributions of K and L shells. This form is based on the superposition of hydrogenic closed-shell momentum densities. Parameters in the form are determined by requiring the zeroth, first, second, and third moments of these distributions to be equal to the corresponding HF results. The hydrogenic model was previously applied to calculate ionization-generalized oscillator strengths using the sum-rule constrained classical-binary-collision model [5,6]. The present work concerns the construction of analytical functions for the momentum-density distributions and Compton profiles for each shell. To the best of our knowledge, no such function for Compton profiles is available except for the helium atom [7].

II. THEORY

The momentum-space atomic wave functions are defined as the Fourier transform of coordinate-space atomic wave functions, i.e.,

$$\phi(\mathbf{p})=\frac{1}{(2\pi)^{3/2}}\int \psi(\mathbf{r})\exp(-i\mathbf{p}\cdot\mathbf{r})d\mathbf{r} \; . \tag{1}$$

In the central-field approximation, Eq. (1) reduces to

$$\phi_{nl}(p)=\left[\frac{2}{\pi}\right]^{1/2}\int_0^\infty r^2 R_{nl}(r)j_l(pr)dr \; , \tag{2}$$

where $R_{nl}(r)$ is the radial part of $\psi(\mathbf{r})$, $j_l(pr)$ is the spherical Bessel function, n is the principal quantum number, and l is the angular-momentum quantum number. The momentum-density distribution for each shell can then be developed using $\phi_{nl}(p)$.

The momentum-density distribution for a closed-shell hydrogenic atom is given by [8]

$$I(p)=4\pi p^2\rho(p)=\frac{32\zeta^5 p^2}{\pi(\zeta^2+p^2)^4} \; , \tag{3}$$

where $\rho(p)$ is the normalized momentum-density distribution, i.e., $\int 4\pi p^2\rho(p)dp=1$, and $\zeta^2/2=E$ is the average kinetic energy of electrons in that shell. Note that atomic units are used throughout this paper. Comparing the average kinetic energy of electrons, i.e., the second moment of the momentum-density distribution, obtained using Slater's rules [9] for the hydrogenic closed shell with corresponding HF data [10], we find that the error is within 2% for the K shell and 6% for the L shell for all atoms. To improve the accuracy of Eq. (3), we propose

$$I_i(p)=4\pi p^2\rho_i(p)=\frac{32}{\pi}\sum_{j=1}^{2}\frac{A_{ij}\zeta_{ij}^5 p^2}{(\zeta_{ij}^2+p^2)^4} \quad (i=K,L) \tag{4}$$

for the ith-shell momentum-density distribution. Here we take A_{ij} and ζ_{ij} as parameters to be determined by requiring several moments of $I_i(p)$ in Eq. (4) to be equal to the corresponding HF results.

TABLE I. Parameters in Eq. (4) for atomic momentum-density distribution of K shell.

Element (Z)	A_{K1}	ζ_{K1}	ζ_{K2}
He (2)	0.8525	1.4913	2.5586
Li (3)	0.8849	2.4761	3.9533
Be (4)	0.9042	3.4634	5.3326
B (5)	0.8989	4.4190	6.5313
C (6)	0.8861	5.3588	7.6444
N (7)	0.8685	6.2866	8.7043
O (8)	0.8507	7.2103	9.7528
F (9)	0.8240	8.1134	10.731
Ne (10)	0.7862	8.9904	11.644
Na (11)	0.7603	9.8862	12.630
Mg (12)	0.7421	10.795	13.651
Al (13)	0.7283	11.711	14.690
Si (14)	0.7170	12.632	15.736
P (15)	0.7099	13.540	16.751
S (16)	0.7066	14.501	17.878
Cl (17)	0.6702	15.360	18.766
Ar (18)	0.6812	16.332	19.917
K (19)	0.6676	17.246	20.922
Ca (20)	0.6719	18.208	22.028
Sc (21)	0.6855	19.202	23.188
Ti (22)	0.6760	20.130	24.205
V (23)	0.6134	20.891	24.915
Cr (24)	0.6653	22.018	26.275
Mn (25)	0.6479	22.919	27.235
Fe (26)	0.6530	23.895	28.332
Co (27)	0.7137	25.063	29.843
Ni (28)	0.6689	25.877	30.565
Cu (29)	0.7009	26.952	31.879
Zn (30)	0.6258	27.637	32.409
Ga (31)	0.5767	28.413	33.156
Ge (32)	0.5693	29.337	34.167
As (33)	0.5767	30.330	35.255
Se (34)	0.6294	31.508	36.645
Br (35)	0.6428	32.526	37.796
Kr (36)	0.5949	33.283	38.522
Rb (37)	0.4484	33.519	38.749
Sr (38)	0.4599	34.540	39.839
Y (39)	0.4491	35.427	40.823
Zr (40)	0.4464	36.360	41.846
Nb (41)	0.4450	37.303	42.873
Mo (42)	0.4420	38.237	43.892
Tc (43)	0.4248	39.082	44.833
Ru (44)	0.4444	40.163	45.969
Rh (45)	0.4359	41.061	46.956
Pd (46)	0.4233	41.922	47.925
Ag (47)	0.4441	43.029	49.063
Cd (48)	0.4537	44.037	50.158
In (49)	0.5085	45.348	51.514
Sn (50)	0.4326	45.810	52.096
Sb (51)	0.4261	46.721	53.089
Te (52)	0.4216	47.640	54.096
I (53)	0.4325	48.683	55.185
Xe (54)	0.4053	49.418	56.064

The mth moment of the ith-shell momentum-density distribution is defined by

$$\langle p^m \rangle_i = \int_0^\infty p^m I_i(p)dp \ . \tag{5}$$

Letting $m=0,1,2,3$ in Eqs. (4) and (5), we get

TABLE II. Parameters in Eq. (4) for atomic momentum-density distribution of L shell.

Element (Z)	A_{L1}	ζ_{L1}	ζ_{L2}
Li (3)	0.9590	0.3994	2.5381
Be (4)	0.9397	0.5648	3.4130
B (5)	0.9404	0.9017	4.1177
C (6)	0.9414	1.2426	4.7817
N (7)	0.9429	1.5831	5.4258
O (8)	0.9421	1.8881	6.0270
F (9)	0.9411	2.2003	6.5902
Ne (10)	0.9401	2.5174	7.1266
Na (11)	0.9447	3.0233	8.0953
Mg (12)	0.9482	3.5191	9.0622
Al (13)	0.9512	4.0133	10.023
Si (14)	0.9534	4.5025	10.958
P (15)	0.9552	4.9895	11.884
S (16)	0.9565	5.4715	12.778
Cl (17)	0.9572	5.9499	13.638
Ar (18)	0.9589	6.4371	14.573
K (19)	0.9599	6.9192	15.457
Ca (20)	0.9621	7.4138	16.458
Sc (21)	0.9611	7.8835	17.167
Ti (22)	0.9609	8.3592	17.933
V (23)	0.9606	8.8346	18.694
Cr (24)	0.9602	9.3077	19.435
Mn (25)	0.9599	9.7816	20.181
Fe (26)	0.9623	10.283	21.878
Co (27)	0.9591	10.724	21.647
Ni (28)	0.9588	11.192	22.289
Cu (29)	0.9589	11.675	23.142
Zn (30)	0.9568	12.128	23.665
Ga (31)	0.9564	12.597	24.379
Ge (32)	0.9561	13.067	25.088
As (33)	0.9554	13.536	25.758
Se (34)	0.9552	14.007	26.461
Br (35)	0.9540	14.473	27.033
Kr (36)	0.9546	14.951	27.860
Rb (37)	0.9548	15.427	28.629
Sr (38)	0.9556	15.911	29.487
Y (39)	0.9546	16.377	30.060
Zr (40)	0.9546	16.854	30.783
Nb (41)	0.9544	17.328	31.473
Mo (42)	0.9544	17.806	32.200
Tc (43)	0.9541	18.281	32.868
Ru (44)	0.9543	18.760	33.619
Rh (45)	0.9543	19.238	34.331
Pd (46)	0.9544	19.718	35.054
Ag (47)	0.9541	20.194	35.718
Cd (48)	0.9548	20.678	36.534
In (49)	0.9542	21.153	37.127
Sn (50)	0.9547	21.637	37.921
Sb (51)	0.9546	22.116	38.605
Te (52)	0.9547	22.597	39.324
I (53)	0.9548	23.079	40.036
Xe (54)	0.9548	23.561	40.746

$$\sum_{j=1}^{2} A_{ij}\zeta_{ij}^{m}=a_m\langle p^m\rangle_i \quad (m=0,1,2,3)\ , \tag{6}$$

where $a_0=1$, $a_1=3\pi/8$, $a_2=1$, and $a_3=3\pi/16$. This procedure guarantees the zeroth, first, second, and third moments of Eq. (4) to be equal to those of the HF momentum-density distribution. Note that the zeroth moment in Eq. (6) is simply the normalization condition, i.e., $A_{i1}+A_{i2}=1$. This condition leaves the number of free parameters in Eq. (4) equal to three. The simultaneous equations of Eq. (6) can be solved for A_{ij} and ζ_{ij} using HF data for $\langle p^m\rangle_i$. Applying HF data for available atoms with Z up to 54 [10], we have solved these equations for the ground-state K and L shells. Solutions are given in Tables I and II.

Under the impulse approximation [11], the isotropic Compton profile of the ith shell, $J_i(q)$, is related to the momentum-density distribution as

$$J_i(q)=\frac{Z_i}{2}\int_q^{\infty}\frac{I_i(p)}{p}dp\ , \tag{7}$$

where Z_i is the occupation number of electrons per atom in the ith shell and q is the projection of electron momentum before the collision on the direction of momentum transfer. Substituting Eq. (4) into Eq. (7), we find the analytical expression for Compton profiles as

$$J_i(q)=\frac{8Z_i}{3\pi}\sum_{j=1}^{2}\frac{A_{ij}\zeta_{ij}^5}{(\zeta_{ij}^2+q^2)^3} \quad (i=K,L)\ . \tag{8}$$

III. RESULTS

Using Eq. (4) with parameters listed in Tables I and II, we have calculated atomic momentum-density distributions of K and L shells. Figure 1 shows a comparison of our results with the corresponding HF data [10] for the K shell of several atoms. Excellent agreement is found for all atoms. The present results (solid curves) and the HF data (dashed curves, but merging into solid curves within graphic scales) agree so closely with each other that one cannot see any difference from the figure. A similar plot for the L shell is shown in Fig. 2. Again, the agreement is so close that only minute differences can be seen. Fig-

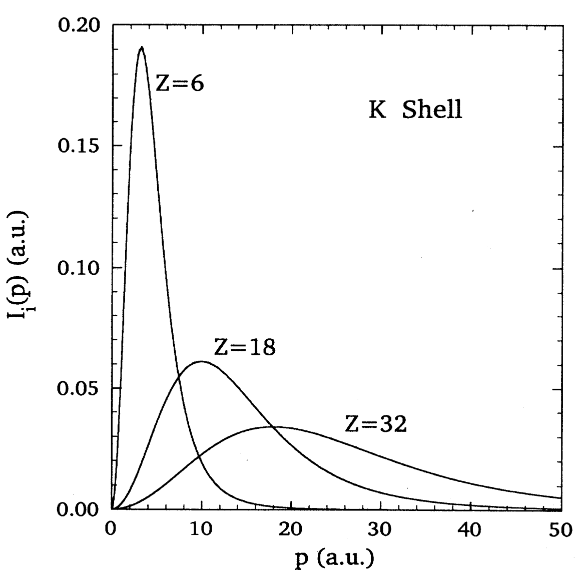

FIG. 1. Plot of the K-shell electron momentum-density distribution for several atoms. Present results (solid curves) are compared to HF data (dashed curves, but coinciding with solid curves within graphic scales) [10]. Atomic units are used.

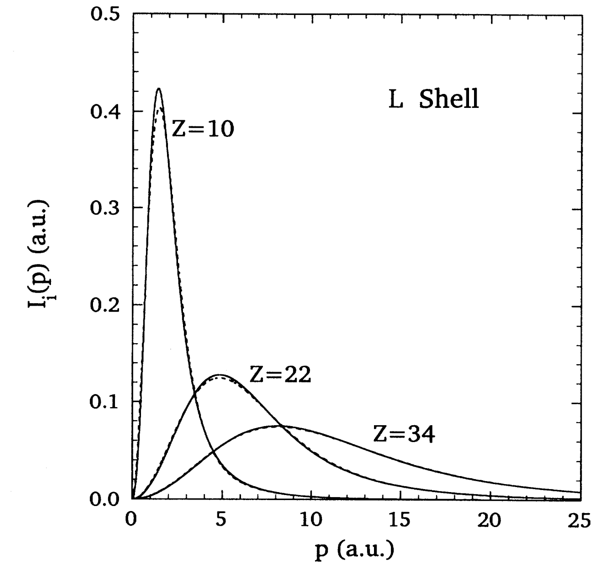

FIG. 2. Plot of the L-shell electron momentum-density distribution for several atoms. Present results (solid curves) are compared to HF data (dashed curves) [10]. Atomic units are used.

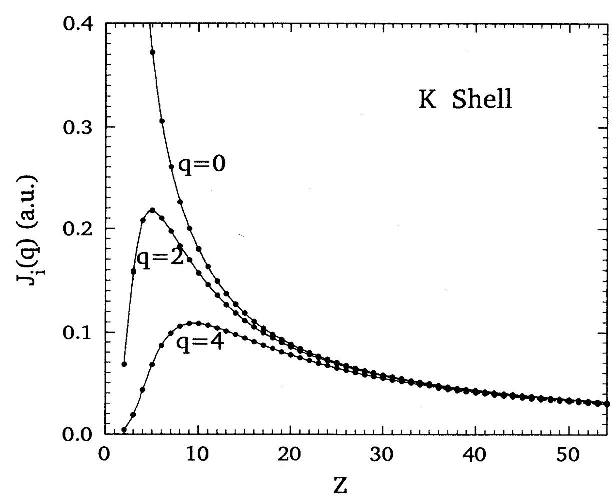

FIG. 3. Plot of the K-shell Compton profile as a function of atomic number for three momentum values. Present results (solid circles) are compared to data calculated using HF wave functions (open circles, but coinciding with solid circles within graphic scales) [12]. The curves are interpolating results showing the dependence of the Compton profile on atomic number. Atomic units are used.

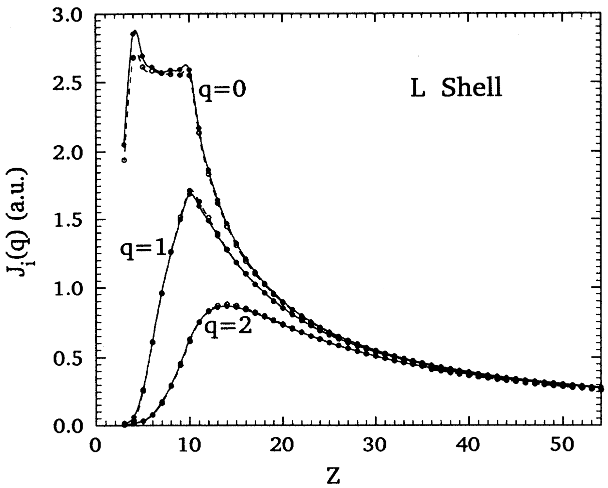

FIG. 4. Plot of the L-shell Compton profile as a function of atomic number for three momentum values. Present results (solid circles) are compared to data calculated using HF wave functions (open circles) [12]. The curves are interpolating results showing the dependence of the Compton profile on atomic number. Atomic units are used.

ure 3 is a plot of the K-shell Compton profile as a function of atomic number for several momentum values. No difference can be seen from the figure between the present results (solid circles) and the HF data (open circles, but merging into solid circles within graphic scales) [12]. Note that all calculated results are plotted as discrete points; interpolating curves serve only to indicate the dependence of these results on atomic number. A similar plot of the L-shell Compton profile is shown in Fig. 4. Still, only minute differences can be seen.

IV. CONCLUSION

In this work, we have constructed simple analytical expressions for the atomic momentum-density distribution and Compton profile of K and L shells. Although it was not discussed, we have calculated the stopping cross section of K and L shells for protons using Eq. (4) and the stopping-power formula [13]. In all these calculations, we found excellent agreement between the present results and detailed theoretical computations.

An extension of this work to other shells seems plausible. However, the superposition of hydrogenic closed-shell momentum densities in Eq. (4) should include more terms. It requires then additional moments in Eq. (5) to be applied. If electrons in the M and higher shells belong to the valence band, a solid-state rather than atomic theory must be employed.

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