Atomic Compton profiles within different exchange-only theories

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Abstract. The impulse Compton Profiles (CPs) $J(q)$ and the $\langle p^n \rangle$ expectation values for some inert gas atoms (He-Kr) are computed and compared within the Harbola-Sahni (HS), Hartree-Fock (HF) theories and a Self-Interaction-Corrected (SIC) density functional model. The Compton profiles for excited states of helium atom are also calculated. While the calculated CPs are found to generally agree, they differ slightly from one another for small values of the Compton parameter q and are in good agreement for large q values. The $\langle p^n \rangle$ expectation values within the three theories are also found to be comparable. The HS formalism is seen to mimic HF reasonably well in the momentum space, establishing the logical consistency of the former.

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In the phenomenon of Compton scattering, the Compton cross-section (of high-energy X-ray or γ-ray photon inelastically scattered by electrons in matter) has a direct bearing on the electron-momentum density. In the so-termed impulse approximation [1] the Compton cross-section is proportional to an experimentally observable quantity, *viz.* the Compton profile (CP), related to the electron momentum density, *vide*

$$J(q) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \gamma(p_x, p_y, q) \mathrm{d}p_x \mathrm{d}p_y. \tag{1}$$

The momentum density $\gamma(\mathbf{p})$ is the diagonal (*i.e.* $\mathbf{p}' = \mathbf{p}$) part of the full, reduced first-order momentum space density matrix $\Gamma_{\mathrm{mom}}^{(1)}(\mathbf{p}|\mathbf{p}')$ connected, in turn, to the many-electron momentum-space wave function [2] $\Phi(\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_N)$ by

$$\Gamma_{\mathrm{mom}}^{(1)}(\mathbf{p}|\mathbf{p}') =$$
$$N \int \Phi^*(\mathbf{p}, \mathbf{p}_2, \ldots, \mathbf{p}_N)$$
$$\times \Phi(\mathbf{p}', \mathbf{p}_2, \ldots, \mathbf{p}_N) \mathrm{d}^3 p_2 \ldots \mathrm{d}^3 p_N, \tag{2}$$

where a sum over spin may also be included.

Within the independent-electron approximation such as the Hartree-Fock (HF) theory, $\Gamma_{\mathrm{mom}}^{(1)}(\mathbf{p}|\mathbf{p}')$ takes the form [3]

$$\Gamma_{\mathrm{mom}}^{(1)}(\mathbf{p}|\mathbf{p}') = \sum_i f_i \phi_i^*(\mathbf{p}) \phi_i(\mathbf{p}'),$$

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with i sweeping through the "occupied" states with the occupancies f_i and $\phi_i(\mathbf{p})$, the momentum-space orbital, being the Fourier transform of the coordinate-space orbital $\psi_i(\mathbf{r})$ related through (Hartree atomic units, employed throughout)

$$\phi_i(\mathbf{p}) = \frac{1}{(2\pi)^{3/2}} \int e^{i\mathbf{p}\cdot\mathbf{r}} \psi_i(\mathbf{r}) \mathrm{d}^3 r. \tag{3}$$

The $\langle p^n \rangle$-moments are defined in terms of electron momentum density (EMD) distribution by

$$\langle p^n \rangle = 4\pi \int_0^{\infty} p^{n+2} \gamma(p) \mathrm{d}p,$$
$$-2 \leq n \leq 4, \tag{4}$$

where $\gamma(p) = \frac{1}{4\pi} \int \gamma(\mathbf{p}) \mathrm{d}\Omega_{\hat{p}}$ is the spherically averaged EMD, in turn leading to the spherically averaged impulse Compton profile $J(q) = 2\pi \int_{|q|}^{\infty} \gamma(p)\, p\, \mathrm{d}p$. These $\langle p^n \rangle$ expectation values sample the interior as well as exterior regions of the EMD and are also related to atomic properties. The $\langle 1/p \rangle$ moment is twice the peak value of the impulse profile $J(0)$; the $\langle p^2 \rangle$ moment is twice the kinetic energy ($= -E_{\mathrm{total}}$, by the virial theorem) while the $\langle p \rangle$ moment is empirically found to be almost proportional to the exact Hartree-Fock exchange energy [4].

The recent Harbola-Sahni approach [5,6] to the atomic structure calculations proffers an attractive alternative to the conventional Hartree-Fock description. The HS approach has been proven to be successful in giving the total energies [7,8] and co-ordinate space

properties [9,10] practically of Hartree-Fock quality. In addition, coupled with local correlation, it also describes the excited states of atoms quite accurately [11]. This success of the HS formalism prompts one for its critical appraisal in the momentum space through Compton profiles and the $\langle p^n \rangle$ expectation values. We also compare these with the corresponding quantities calculated within the HF, the HS and the self-interaction-corrected (SIC) local density functional theories. This study is aimed at bringing out how these **p**-space quantities calculated using the *local* and *orbital-independent* prescription of HS compare with those of the HF theory, which employs a nonlocal potential (in its *exact* exchange description), and of SIC theory in which the effective potential, although local, turns out to be orbital-dependent. In the following we first briefly describe the HF, HS and SIC theories to highlight the differences among them.

All the three theories HF, HS and SIC are independent particle theories in which the electron orbitals are obtained by solving the equations (Hartree atomic units, *i.e.* $\hbar = |e| = m = 1$ are used throughout herein), *viz.*

$$\left[-\frac{\nabla^2}{2} + v_{\mathrm{H}}(\mathbf{r}) + v_x(\mathbf{r}) \right] \psi_i = \epsilon_i \psi_i;$$
$$i = 1, 2, \ldots N, \qquad (5)$$

where $v_{\mathrm{H}}(\mathbf{r}) = v_{\mathrm{nuclear}}(\mathbf{r}) + \int \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \mathrm{d}^3 r'$ is the Hartree potential and v_x the exchange potential. Here $\rho(\mathbf{r})$ is the electronic density given in terms of orbitals $\psi_i(\mathbf{r})$ as $\rho(\mathbf{r}) = \sum_i f_i |\psi_i(\mathbf{r})|^2$. The differences in HF, HS and SIC precisely lie in the manner in which the exchange potential is prescribed in them. In HF, which is the exact theory at the "exchange-only" level, as noted above, the potential v_x is *nonlocal* with its action on $\psi_i(\mathbf{r})$ given by

$$v_x(\mathbf{r})\psi_i(\mathbf{r}) =$$
$$\sum_{\substack{j \\ \mathrm{spin}\, i = \mathrm{spin}\, j}} \int \frac{\psi_j^*(\mathbf{r}')\psi_j(\mathbf{r})\psi_i(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \mathrm{d}^3 r'. \qquad (6)$$

On the other hand, the exchange potential in the exchange-only HS theory is local and is prescribed as the work done in moving an electron in the field of its Fermi hole [5]:

$$v_x(\mathbf{r}) = W_x(\mathbf{r}) = -\int_\infty^{\mathbf{r}} \mathcal{E}_x \cdot \mathrm{d}\mathbf{l}, \qquad (7)$$

where

$$\mathcal{E}_x(\mathbf{r}) = \int \frac{\rho_x(\mathbf{r},\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|^3} (\mathbf{r} - \mathbf{r}') \, \mathrm{d}^3 r' \qquad (8)$$

is the exchange "electric field" due to the Fermi hole (or the "exchange hole") $\rho_x(\mathbf{r},\mathbf{r}')$.

In the SIC theory the exchange potential is calculated within the local-density approximation (LDA) which is

Table 1. Spherically averaged Compton profile, $J_{\mathrm{sph}}(q)$ for helium within the three "exchange-only" theories compared with their experimental counterpart. (Hartree a.u. used throughout.)

q	HF	HS	SIC	Experiment [a]
0.0	1.070	1.070	1.070	1.071±1.5%
0.2	1.017	1.017	1.017	1.019
0.6	0.700	0.700	0.700	0.705
1.0	0.382	0.382	0.382	0.388
1.5	0.160	0.160	0.160	–
2.0	0.068	0.068	0.068	0.069
2.5	0.031	0.031	0.031	0.030±15%
3.0	0.015	0.015	0.015	0.013

[a] Reference [18].

Table 2. $J_{\mathrm{sph}}(q)$ for neon.

q	HF	HS	SIC	CI[a]	Experiment[b]
0.0	2.727	2.719	2.751	2.739	2.762
0.2	2.696	2.687	2.717	2.707	2.738
0.4	2.593	2.585	2.608	2.602	2.630
0.6	2.413	2.406	2.418	2.4159	2.427
0.8	2.168	2.162	2.163	2.1645	2.162
1.0	1.889	1.885	1.875	1.880	1.859
1.5	1.228	1.228	1.211	–	–
2.0	0.771	0.774	0.764	0.768	0.765
2.5	0.501	0.506	0.501	–	0.501
3.0	0.346	0.350	0.349	0.348	0.359
3.5	0.253	0.256	0.256	–	0.277
4.0	0.194	0.196	0.197	0.196	0.210
5.0	0.125	0.125	0.126	0.126	0.126

[a] Reference [20].
[b] Reference [19].

then *ad hoc* corrected for its self-interaction on an orbital-by-orbital basis [12]. Thus the *orbital-dependent* SIC exchange potential is given as

$$v_{\mathrm{SIC},x}^i(\mathbf{r}) = \left(\frac{-3}{4} \right) \left(\frac{3}{\pi} \right)^{1/3} \rho^{1/3}(\mathbf{r})$$
$$- \left\{ \int \frac{|\psi_i(\mathbf{r}')|^2}{|\mathbf{r}-\mathbf{r}'|} \mathrm{d}^3 r' + \left(\frac{-3}{4} \right) \left(\frac{6\rho_i(\mathbf{r})}{\pi} \right)^{1/3} \right\}, \quad (9)$$

where $\rho_i(\mathbf{r}) = |\psi_i(\mathbf{r})|^2$ is the orbital density.

In the context of HS potential, it may be noted that as recently established by Holas and March [13], the Harbola-Sahni exchange-correlation potential can also be calculated from the exact second-order density matrix by employing the differential virial theorem. The results are consistent with, and provide the mathematical proof of the formalism proposed by HS. In addition, it also spells out how the kinetic-energy term missing [5,6] from the HS potential arises from the differences in the exact kinetic-energy density tensor and its

Table 3. $J_{\mathrm{sph}}(q)$ for argon.

q	HF	HS	SIC	Experiment[a]
0.0	5.064	5.040	5.093	5.058
0.2	4.963	4.941	4.991	4.917
0.4	4.619	4.605	4.638	4.526
0.6	4.035	4.029	4.033	3.960
0.8	3.333	3.331	3.312	3.319
1.0	2.661	2.664	2.636	2.697±1%
1.5	1.546	1.557	1.540	–
2.0	1.084	1.090	1.086	1.129
2.5	0.874	0.876	0.875	0.904
3.0	0.736	0.736	0.737	0.744
3.5	0.622	0.621	0.620	0.634
4.0	0.520	0.519	0.520	0.534±2.5%
4.5	0.433	0.432	0.432	–
5.0	0.359	0.359	0.359	0.366
10.0	0.075	0.076	0.076	0.078±10%
15.0	0.025	0.025	0.025	0.025

[a] Reference [18].

Table 4. $J_{\mathrm{sph}}(q)$ for krypton.

q	HF	HS	SIC	Experiment[a]
0.0	7.237	7.195	7.262	7.188
0.2	7.095	7.060	7.122	6.988
0.4	6.605	6.586	6.625	6.453
0.6	5.785	5.781	5.783	5.702
0.8	4.855	4.863	4.841	4.883
1.0	4.044	4.059	4.032	4.131±1.7%
2.0	2.442	2.447	2.448	2.557
3.0	1.858	1.857	1.854	–
4.0	1.327	1.324	1.319	1.350
5.0	0.935	0.935	0.931	0.933±3.5%
10.0	0.260	0.260	0.261	0.254
15.0	0.105	0.105	0.105	0.099

[a] Reference [18].

Table 5. $\langle p^n \rangle$ moments for helium within different "exchange-only" theories.

Moments	HF	HS	SIC
$\langle p^{-2} \rangle$	$4.0893 \cdot 10^0$	$4.0760 \cdot 10^0$	$4.0902 \cdot 10^0$
$\langle p^{-1} \rangle$	$2.1406 \cdot 10^0$	$2.1409 \cdot 10^0$	$2.1410 \cdot 10^0$
$\langle p \rangle$	$2.7990 \cdot 10^0$	$2.7990 \cdot 10^0$	$2.7987 \cdot 10^0$
$\langle p^2 \rangle$	$5.7234 \cdot 10^0$	$5.7234 \cdot 10^0$	$5.7138 \cdot 10^0$
$\langle p^3 \rangle$	$1.7991 \cdot 10^1$	$1.7990 \cdot 10^1$	$1.7628 \cdot 10^1$
$\langle p^4 \rangle$	$1.0567 \cdot 10^2$	$1.0549 \cdot 10^2$	$8.7395 \cdot 10^2$

Table 6. $\langle p^n \rangle$ moments for neon.

Moments	HF	HS	SIC
$\langle p^{-2} \rangle$	$5.4795 \cdot 10^0$	$5.4526 \cdot 10^0$	$5.6349 \cdot 10^0$
$\langle p^{-1} \rangle$	$5.4558 \cdot 10^0$	$5.4387 \cdot 10^0$	$5.5025 \cdot 10^0$
$\langle p \rangle$	$3.5196 \cdot 10^1$	$3.5269 \cdot 10^1$	$3.5246 \cdot 10^1$
$\langle p^2 \rangle$	$2.5709 \cdot 10^2$	$2.5708 \cdot 10^2$	$2.5771 \cdot 10^2$
$\langle p^3 \rangle$	$3.5843 \cdot 10^3$	$3.5720 \cdot 10^3$	$3.5836 \cdot 10^3$
$\langle p^4 \rangle$	$9.8510 \cdot 10^4$	$9.9418 \cdot 10^4$	$9.9898 \cdot 10^4$

Table 7. $\langle p^n \rangle$ moments for argon.

Moments	HF	HS	SIC
$\langle p^{-2} \rangle$	$1.3107 \cdot 10^1$	$1.2943 \cdot 10^1$	$1.3253 \cdot 10^1$
$\langle p^{-1} \rangle$	$1.0128 \cdot 10^1$	$1.0076 \cdot 10^1$	$1.0187 \cdot 10^1$
$\langle p \rangle$	$8.8699 \cdot 10^1$	$8.8796 \cdot 10^1$	$8.8793 \cdot 10^1$
$\langle p^2 \rangle$	$1.0536 \cdot 10^3$	$1.0536 \cdot 10^3$	$1.0538 \cdot 10^3$
$\langle p^3 \rangle$	$2.4301 \cdot 10^4$	$2.4307 \cdot 10^4$	$2.3997 \cdot 10^4$
$\langle p^4 \rangle$	$1.1393 \cdot 10^6$	$1.1723 \cdot 10^6$	$5.4391 \cdot 10^6$

Slater-Kohn-Sham orbitals counterpart [13]. Similar analysis carried out within the Hartree-Fock theory [14] reveals that the difference between the exact KS exchange-only potential and the HS potential is traced back to the differences in the kinetic-energy density tensors of the HF theory and its local counterpart (as such, this difference is indeed only marginal) [14]. Further, within a local prescription, it is not clear as to how one incorporates the kinetic-energy effects directly in a self-consistent-field (SCF) scheme.

In this work the spherically averaged Compton profiles $J(q)$ within the HF theory are computed using the near Hartree-Fock (NHF) quality wave functions that employ the STO (Slater-Type-Orbital) bases tabulated by Clementi and Roetti [15] and the values of the $\langle p^n \rangle$ moments are from ref. [16]. On the other hand, the orbitals with effective potential W_x are obtained by a modified Herman-Skillman code [17]. The calculated Compton pro-

files along with their available experimental [18,19] and accurate theoretical counterparts [20] are tabulated in Tables 1-4 for inert atomic systems He-Kr while the moments are displayed in Tables 5-8. The helium atom in its ground state has a single orbital, hence all the CPs within these three exchange-only theories practically coincide (cf. Tab. 1). For Ne, Ar and Kr, it is evident from Tables 2-5 that for *low* q-values the CPs differ from each other appreciably. For higher q-values these theoretical (HF, HS, SIC) profiles are in better agreement with one another. In the low-q region ($q < 0.5$ au), the SIC profiles are seen to be the largest and the HS profiles are the smallest in magnitude among the three theories. Beyond $q \sim 0.5$ a.u. the three profiles cross each other and are in good agreement in the asymptotic region. It is observed further that the "experimental" $J(q)$ is fairly well estimated by the "exchange-only" theories. It is to be noted that an accurate theoretical $J(q)$ computation beyond HF, *viz.* the configuration interaction calculation for *Ne*, due to Tripathi *et al.* [20] while improving upon the HF-CP still slightly underestimates the experimental $J(0)$ but overestimates the intermediate profile. The higher values of $J(q)$ in the SIC theory indicate that the momentum density is

Table 8. $\langle p^n \rangle$ moments for krypton.

Moments	HF	HS	SIC
$\langle p^{-2} \rangle$	$1.7478 \cdot 10^1$	$1.7084 \cdot 10^1$	$1.7517 \cdot 10^1$
$\langle p^{-1} \rangle$	$1.4474 \cdot 10^1$	$1.4390 \cdot 10^1$	$1.4524 \cdot 10^1$
$\langle p \rangle$	$2.8141 \cdot 10^2$	$2.8161 \cdot 10^2$	$2.8155 \cdot 10^2$
$\langle p^2 \rangle$	$5.5041 \cdot 10^3$	$5.5013 \cdot 10^3$	$5.5072 \cdot 10^3$
$\langle p^3 \rangle$	$2.2628 \cdot 10^5$	$2.2424 \cdot 10^5$	$2.2453 \cdot 10^5$
$\langle p^4 \rangle$	$1.9852 \cdot 10^8$	$5.0212 \cdot 10^7$	$5.0297 \cdot 10^7$

Table 9. $J_{\mathrm{sph}}(q)$ for different states of helium atom within the Harbola-Sahni approach.

q	$1s^2$	$1s2s$	$1s2p$	$1s3p$	$1s4p$
0.0	1.070	2.516	1.583	2.966	4.433
0.2	1.017	1.532	1.467	1.266	0.955
0.4	0.879	0.592	0.949	0.517	0.423
0.6	0.700	0.362	0.537	0.412	0.357
0.8	0.527	0.294	0.340	0.303	0.287
1.0	0.382	0.237	0.239	0.228	0.223
1.5	0.160	0.119	0.111	0.112	0.111
2.0	0.068	0.056	0.052	0.053	0.053
2.5	0.031	0.029	0.025	0.025	0.025
3.0	0.015	0.013	0.012	0.012	0.012

localized near the origin $\mathbf{p} = \mathbf{0}$ in the SIC formalism. This can also be seen from the $\langle p^{-2} \rangle$ and $\langle p^{-1} \rangle$ values which, as pointed out above, sample the interior region of the EMD. The higher the momentum density near the origin the greater the values of these moments. That these moments have largest values in the SIC formalism may be qualitatively explained as follows: The region near the origin in the momentum space by Fourier reciprocity corresponds to the asymptotic region in the position space. In the density functional theory (DFT) the asymptotic decay of the co-ordinate space electron density goes as $\sim \exp(-2\sqrt{2|\epsilon_{\max}|}\, r)$, where $\epsilon_{\max}$ is the eigenvalue of the highest occupied orbital [21]. The highest occupied orbital energy eigenvalues for these systems in the SIC formalism are smaller in magnitude compared to their HF and HS counterparts. Consequently, the coordinate-space electron density decays more slowly in SIC than in the HS and HF theories, leading therefore to higher values of $\langle p^{-2} \rangle$ and $\langle p^{-1} \rangle$ moments. The larger values of the HF profiles than HS profiles near $q = 0$ can also be explained similarly. In the HF theory (unlike in DFT), *all* the orbitals decay with the same exponent $(\sim \exp(-\sqrt{2|\epsilon_{\mathrm{HF}}^{\max}|}\, r))$ asymptotically ($\epsilon_{\mathrm{HF}}^{\max}$ here is the highest occupied HF orbital energy eigenvalue) [22] which, by reciprocity, reflects in the slower decay of $\gamma(\mathbf{p})$ in the small $|\mathbf{p}|$, resulting therefore in slightly larger values of $\langle 1/p^2 \rangle$, $\langle 1/p \rangle$ moments and $J_{\mathrm{HF}}(q)$ (near $q = 0$) as compared to their HS counterparts. Amongst the various moments, the agreement among these theories is the best for the $\langle p^2 \rangle$ moments. The HF and HS values of this moment are very close, agreeing up to four

significant figures in case of Ne and Ar, and up to three significant figures for Kr. This agreement is however not surprising since this moment is essentially the double of the negative of the total energy (by the virial theorem) and the HS theory is known to produce the total energies which are practically equivalent to their HF counterparts. Further, the $\langle p \rangle$ and $\langle p^3 \rangle$ moments are also found to be comparable in the three theories. The $\langle p^4 \rangle$ moments within HS agree with their corresponding HF and/or SIC values. Thus, the HS theory with its local prescription for the exchange potential is seen to mimic the Hartree-Fock formalism reasonably well in the momentum space. Our study on the detailed structure of the radially projected first-order reduced density matrix [3] also supports this similarity between the HS and HF density matrices: striking similarities are observed in the structure (contours) of reduced first-order density matrix in the momentum space.

The HS theory also offers a simpler description of the bound excited states in comparison with the HF description. This is because the HS formalism is not based on the variational principle, but rather on the physical effect of the Pauli and Coulomb correlations; which has prompted us to compute the CPs for the excited states of helium. Of course, the numerical HF approach is also perfectly suitable for excited states with the orbitals identified from the number of radial nodes $(= n - l - 1)$ of a given radial part $R_{nl}(r)$ of the orbital. However, the appeal of the HS approach is that it is much simpler to implement than the numerical HF scheme, yielding results that are practically equivalent to the latter. The CPs calculated for various excited states of helium are presented in Table 9. The excited states of helium atom will have diffused electron distribution in the position space and also will have higher total energy. Consequently, the excited-state CPs will be more compact or localized in the small-q region, as is evident from Table 9.

One naively expects that the HS Compton profiles may be improved by adding an accurate local correlation to its effective potential. It is observed, however, that addition of an *ad hoc* correlation (such as the Gunnarsson-Lundqvist [23] or Ceperly-Alder [12] prescriptions) to the effective HS potential results in an undesirable lowering of the peak profile. If the correlation is added right at the level of the exchange-correlation hole (ρ_x replaced by ρ_{xc} in equation (8)) and *then* the HS computations are performed self-consistently, an improvement over the

"exchange-only" $J(q)$ is expected. On the other hand, though the work of Holas and March [13], as pointed above, prescribes an inclusion of the kinetic piece of correlation in the KS context, it is not known how one actually implements their scheme in practice. These studies, of course, go beyond the scope of the present "exchange-only" theme.

In this paper, we have carried out a comparative study of the momentum space properties of atoms *viz.* Compton profiles and various expectation values calculated within the "work formalism" of Harbola and Sahni, the Hartree-Fock theory as well as the Self-Interaction-Corrected local-density approximation theory. The Compton profiles for various excited states of the helium atoms are also presented within the work formalism. The present work demonstrates that the Harbola-Sahni work formalism which in position space closely follows the HF theory is also seen to do so in the momentum space, bringing out the logical consistency of the HS theory.

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