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Compton profiles of atoms from electron densities via reciprocal form factors

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Abstract. A new method to extract the Compton profile from the electron density has been proposed. The method is based on the nonlocal density approximation (NLDA) due to Gunnarsson *et al* and Alonso and Girifalco. Initially the reduced first order density matrix has been estimated from the knowledge of the electron density alone through the use of an averaged density distribution, $\tilde{\rho}(r)$. The reduced first order density matrix thus obtained has then been employed to extract the reciprocal form factor, $B(r)$. The Compton profile, $J(q)$ may thereby be obtained by a cosine transformation of $B(r)$. These results for the $J(q)$ are in good agreement with their near Hartree-Fock counterparts.

Keywords. Compton profile; reciprocal form factor; electron density; electron momentum density; density matrix.

1. Introduction

The study and measurements of Compton profiles have received a good deal of attention in the past decade or so. The reason for such an interest is that with the advent of intense γ-ray and synchrotron radiation sources very accurate determination of the momentum space properties of electrons in the sample has become possible. Extensive reviews both of theoretical and experimental aspects of Compton scattering and related techniques are available (Williams 1977a, b). The Compton profile is related to the spherically averaged electron momentum density, $\gamma(p)$ via the relation:

$$J(q) = 2\pi \int_{|q|}^{\infty} \gamma(p)\, p\, dp, \tag{1}$$

where q is the projection of an electron's initial momentum onto the scattering vector. Reciprocally,

$$\gamma(p) = \frac{-1}{2\pi} p^{-1} \frac{dJ(q)}{dq}\bigg|_{q=p}. \tag{2}$$

Various other properties viz. the $\langle p^n \rangle$-values may be extracted from the Compton profiles (Benesch and Smith 1973).

$$\langle p^n \rangle = 2(n+1) \int_0^{\infty} J(q) q^n dq, \quad 0 \leqslant n \leqslant 4, \tag{3}$$

Dedicated to Professor Sadhan Basu on the occasion of his 65th birth anniversary.

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the $\langle p^{-1} \rangle$ is related to the peak height of the Compton profile by

$$\langle p^{-1} \rangle = 2\,J(0). \tag{4}$$

However, analysis and interpretation of Compton profiles is not limited to momentum space only. The Fourier transform of the Compton profile viz. the reciprocal form factor, $B(\mathbf{r})$ has been found (Weyrich *et al* 1979) to be a convenient tool to study and interpret simple chemical concepts such as hybridization, and bonding. The spherically averaged $B(r)$ is given by (Thakkar *et al* 1983):

$$B(r) = 2\int_0^\infty J(q)\cos(qr)\,\mathrm{d}r. \tag{5}$$

The first order reduced density matrix is related to $B(r)$ via the relations (Thakkar *et al* 1983),

$$B(\mathbf{r}) = \int \Gamma(\mathbf{s}/\mathbf{s}+\mathbf{r})\,\mathrm{d}\mathbf{s}, \tag{6}$$

and

$$B(r) = 1/4\pi \int B(\mathbf{r})\,\mathrm{d}\Omega. \tag{7}$$

Thus the $B(r)$ function emerges as a convenient bridge between the coordinate and momentum spaces.

The reduced first order density matrices in configuration and momentum space are related to each other by (Benesch and Smith 1973),

$$\Gamma(\mathbf{p}/\mathbf{p}') = [1/(2\pi)^3] \int \Gamma(\mathbf{r}/\mathbf{r}')\,e^{-i\mathbf{p}\cdot\mathbf{r}} e^{i\mathbf{p}'\mathbf{r}'}\,\mathrm{d}\mathbf{r}\mathrm{d}\mathbf{r}'. \tag{8}$$

The electron momentum density, $\gamma(p)$ is the diagonal component of $\Gamma(\mathbf{p}/\mathbf{p}')$ i.e.

$$\gamma(\mathbf{p}) = \Gamma(\mathbf{p}/\mathbf{p}') \tag{9}$$

and the spherically averaged momentum density is given by

$$\gamma(p) = (1/4\pi) \int \gamma(\mathbf{p})\mathrm{d}\Omega. \tag{10}$$

The electron density, $\rho(\mathbf{r})$ may be defined in a similar manner. Unfortunately, the transformation from ρ to γ and the converse is not as yet available contrary to the one between the density matrices as defined by (8). Thus it is necessary to resort to certain approximate procedures to extract momentum density from the electron density and vice versa. The currently available procedures are the ones due to Lam and Platzman (1974), viz., the locally averaged method, (LAM) and Gadre and Pathak (1981), which basically employs semiclassical considerations as those adopted by Burkhardt (1936), Kònya (1949), Coulson and March (1950) (BKCM). Later Pathak *et al* (1983) enforced the constraint of the kinetic energy to the $\gamma(p)$ obtained from the BKCM method. Though there is some improvement in the $\gamma(p)$ predicted, the results are far from acceptable. Recently, Gadre and Chakravorty (1986) proposed leading and tail corrections to the BKCM model. This leads to drastic improvement over some of the momentum space

properties. However, the methods proposed do not yield sufficiently accurate estimates of all properties in momentum space.

In the present work, a new method to determine the Compton profile from the knowledge of electron density alone, is presented. To start with, an approximate reduced first order density matrix in coordinate space is constructed from which the Compton profile is subsequently extracted via the reciprocal form factor.

2. Method

The first order reduced density matrix in coordinate space may be written as (Deb and Ghosh 1983; Ludeña 1983a, b):

$$\Gamma(\mathbf{r}/\mathbf{r}') = \rho^{1/2}(\mathbf{r})\,\rho^{1/2}(\mathbf{r}')\,G(\mathbf{r},\mathbf{r}'), \tag{11}$$

where $G(\mathbf{r},\mathbf{r}')$ satisfies the condition,

$$G(\mathbf{r},\mathbf{r}) = 1. \tag{12}$$

Using an orbital expansion, $G(\mathbf{r},\mathbf{r}')$ may be written as

$$G^2(\mathbf{r},\mathbf{r}') = \left[\sum_{i=1}^{n}\sum_{j=1}^{n} \phi i^*(\mathbf{r})\phi_i(\mathbf{r}')\,\phi_j^*(\mathbf{r})\,\phi_j(\mathbf{r}')\right] \Bigg/ \left[\sum_{i=1}^{n} \phi_i^*(\mathbf{r})\,\phi_i(\mathbf{r}) \sum_{j=1}^{n} \phi_j(\mathbf{r}')\,\phi_j(\mathbf{r}')\right]. \tag{13}$$

Substituting plane waves for ϕ_i's the homogeneous electron gas pair correlation function is obtained (Deb and Ghosh 1983; Ludenã 1983a, b):

$$G(\mathbf{r},\mathbf{r}') = 3\,j_1(y)/y, \tag{14}$$

where $j_1(y)$ is the first order spherical Bessel function:

$$j_1(y) = [\sin(y) - y\cos(y)]/y^2, \tag{15}$$

with $y = k_f|\mathbf{r}-\mathbf{r}'|$ and k_f = the Fermi momentum.

Another approach to determine an approximate relationship between $\rho(\mathbf{r})$ and the $\Gamma(\mathbf{r}/\mathbf{r}')$ was employed by Gunnarsson *et al* (1976, 1977) and Alonso and Girifalco (1977, 1978). The two particle spinless density matrix, $\Gamma(\mathbf{r},\mathbf{r}'/\mathbf{r},\mathbf{r}')$ is given by

$$\Gamma(\mathbf{r},\mathbf{r}'/\mathbf{r},\mathbf{r}') = \rho(\mathbf{r})\rho(\mathbf{r}') - 1/2\,\Gamma(\mathbf{r}/\mathbf{r}')\,\Gamma(\mathbf{r}'/\mathbf{r}), \tag{16}$$

using the relation

$$\Gamma(\mathbf{r},\mathbf{r}'/\mathbf{r},\mathbf{r}') = \rho(\mathbf{r})\,\rho(\mathbf{r}')[1 + C(\mathbf{r},\mathbf{r}')]. \tag{17}$$

$C(\mathbf{r},\mathbf{r}')$ is the correlation factor which is known exactly for a homogeneous electron gas (Gunnarsson *et al* 1976, 1977; Alonso and Girifalco 1977, 1978).

$$C(\mathbf{r},\mathbf{r}') = (-9/2)[j_1^2(y)/y^2] \tag{18}$$

with $y = k_f|\mathbf{r}-\mathbf{r}'|$. Thus, comparing (11), (16), (17) and (18), the relation between $C(\mathbf{r},\mathbf{r}')$ and $G(\mathbf{r},\mathbf{r}')$ is given by,

$$G(\mathbf{r},\mathbf{r}') = [-2\,C(\mathbf{r},\mathbf{r}')]^{1/2}, \tag{19}$$

which is the same expression as (14). In the local density approximation it is assumed that

$$\rho(\mathbf{r}) = \rho(\mathbf{r}'), \tag{20a}$$

leading to

$$k_f(\mathbf{r}) = [3\pi^2\rho(\mathbf{r})]^{1/3}. \tag{20b}$$

However, it may be noted that the assumption (20a) is a very drastic one, especially for the atomic and molecular case. This serious defect of the LDA (local density approximation) model necessitated an alternative definition (Gunnarsson *et al* 1976, 1977; Alonso and Girifalco 1977, 1978) of $k_f(\mathbf{r})$ resulting in the non local density approximation (NLDA). This was achieved by rejecting the approximation (20a) and replacing the $\rho(\mathbf{r})$ in (20b) by an average density $\tilde{\rho}(\mathbf{r})$ determined by a constraint that the exchange charge density should be conserved (Gunnarsson *et al* 1976, 1977; Alonso and Girifalco 1977, 1978). That means

$$\int \rho(\mathbf{r}) C\tilde{\rho}(\mathbf{r}, \mathbf{r}')\, d\mathbf{r}' = -\mathbf{1}; \tag{21}$$

the new correlation factor $C\tilde{\rho}(\mathbf{r}, \mathbf{r}')$ is

$$C\tilde{\rho}(\mathbf{r}, \mathbf{r}') = (-9/2)[j_1^2(\tilde{y})/\tilde{y}^2], \tag{22}$$

where $\tilde{y} = |\mathbf{r} - \mathbf{r}'|[3\pi^2\tilde{\rho}(\mathbf{r})]^{1/3} = \tilde{k}_f(r)|\mathbf{r} - \mathbf{r}'|$. Thus $\tilde{\rho}(\mathbf{r})$ is determined by solving (21). Another approximation that restores the symmetry of the density matrix is $k_f = [3\pi^2\rho(|\mathbf{r} - \mathbf{r}'|)]^{1/3}$, which will also be examined.

Thus now with an approximate density matrix being constructed from the electron density, $\rho(\mathbf{r})$ the reciprocal form factor, $B(\mathbf{r})$ may be easily obtained employing (6):

$$\Gamma(\mathbf{r}_1/\mathbf{r}_2) = \rho^{1/2}(\mathbf{r}_1)\rho^{1/2}(\mathbf{r}_2)\, 3j_1(x)/x, \tag{23}$$

where $x = y = k_f(\mathbf{r}_1)|\mathbf{r}_1 - \mathbf{r}_2| = [3\pi^2\rho(\mathbf{r}_1)]^{1/3}|\mathbf{r}_1 - \mathbf{r}_2|$ in the LDA model and $x = \tilde{y} = \tilde{k}_f(\mathbf{r}_1)|\mathbf{r}_1 - \mathbf{r}_2| = [3\pi^2\tilde{\rho}(\mathbf{r}_1)]^{1/3}|\mathbf{r}_1 - \mathbf{r}_2|$ in the NLDA model. In the case of atoms, where $\rho(\mathbf{r}) = \rho(r)$ is a reasonable assumption, the $\Gamma(\mathbf{r}_1/\mathbf{r}_2)$ then simplifies to just a function of r_1, r_2 and $|\mathbf{r}_1 - \mathbf{r}_2| = r$. With this simplification the $B(r)$ as in (6) and (7) may be obtained by a suitable transformation to metric coordinates as utilised by Coulson and Neilson (1961).

$$B(r) = \frac{2\pi}{r}\left\{\int_0^r \rho^{1/2}(r_1)\frac{3j_1(x)}{x} r_1 dr_1 \int_{r-r_1}^{r+r_1} \rho^{1/2}(r_2)\, r_2 dr_2 + \right.$$
$$\left. + \int_r^\infty \rho^{1/2}(r_1)\frac{3j_1(x)}{x} r_1\, dr_1 \int_{r_1-r}^{r_1+r} \rho^{1/2}(r_2)\, r_2 dr_2 \right\} = \frac{2\pi}{r} f(r). \tag{24}$$

Within the NLDA model the determination of $\tilde{\rho}(r_1)$ via (21) and (22) remains a cumbersome three-dimensional exercise:

$$1 = (9/2)\int \rho(r_2) j_1^2(\tilde{y})/\tilde{y}^2\, d\mathbf{r}_2. \tag{25}$$

Equation (25) can be further simplified by transforming to metric coordinates (Coulson

and Neilson 1961) viz. r_1, r_2, $|\mathbf{r}_1 - \mathbf{r}_2| = r$ yielding

$$1 = \frac{9\pi}{r_1}\left\{\int_0^{r_1} \rho(r_2)\, r_2\, dr_2 \int_{r_1 - r_2}^{r_1 + r_2} \frac{j_1^2(\tilde{y})}{\tilde{y}^2} r dr + \right.$$

$$\left. + \int_{r_1}^{\infty} \rho(r_2)\, r_2\, dr_2 \int_{r_2 - r_1}^{r_1 + r_2} \frac{j_1^2(\tilde{y})}{\tilde{y}^2} r dr \right\}. \tag{26}$$

Now consider the following indefinite integral

$$3\int \frac{j_1^2(\tilde{y})}{\tilde{y}^2} r dr = 3\int \frac{j_1^2(\tilde{k}_f r)}{\tilde{k}_f^2 r} dr. \tag{27}$$

Employing recurrence relations (Antosiewicz 1970) and integrating (Gradshteyn and Ryzhik 1980, p. 634) one obtains,

$$3\int \frac{j_1^2(\tilde{y})}{\tilde{y}^2} r dr = r^2\left\{\frac{j_0^2(\tilde{y})}{2} - j_{-1}(\tilde{y}) j_1(\tilde{y}) - \frac{j_1^2(\tilde{y})}{4} - \frac{j_0(\tilde{y}) j_2(\tilde{y})}{3} - \frac{j_2^2(\tilde{y})}{12}\right\}$$

$$= g(r_1, r). \tag{28}$$

The above solution is an even function of r, thus (26) simplifies after substitution of (28) in (26) to

$$1 = \frac{3\pi}{r_1}\int_0^{\infty} \rho(r_2)\, r_2 [g(r_1, r)]_{r_1 - r_2}^{r_1 + r_2} dr_2, \tag{29}$$

where $\tilde{y} = [3\pi^2 \tilde{\rho}(r)]^{1/3} r$. Equation (29) offers a direct method for determination of $\tilde{\rho}$. The above simplification has not been utilised (Deb and Ghosh 1983; Ludeña 1983a, b; Gunnarsson *et al* 1976, 1977; Alonso and Girifalco 1977, 1978) nor pointed out earlier in the literature.

3. Relationships

The $B(r)$ obtained from (24) satisfies certain important conditions. For instance, $B(0) = N$, the number of electrons. This can be verified for (24) employing the differentiation formula for a definite integral [pp. 1098, equation (12·211) of (Gradshteyn and Ryzhik 1980)] and L'Hospital's rule. $B(0)$ is given by

$$B(0) = 2\pi f'(r)|_{r=0} = \int_r^{\infty} \rho^{1/2}(r_1) \frac{3j_1(x)}{x} r_1 dr_1 [\rho^{1/2}(r_1 + r)\cdot(r_1 + r) +$$

$$+ \rho^{1/2}(r_1 - r)(r_1 - r)] \tag{30}$$

Thus,

$$B(0) = 4\pi \int_0^{\infty} \rho r^2 dr = N. \tag{31}$$

Recently Thakkar *et al* (1983) have pointed out that the various momentum space properties could be extracted from the knowledge of $B(r)$ alone. For example, the second moment of the electron momentum density which is twice the kinetic energy is given by

$$\langle p^2 \rangle = -3 \frac{d^2 B(r)}{dr^2}\bigg|_{r=0} \tag{32}$$

The $\langle p^2 \rangle$-value for the present transformation can be easily determined employing (24) and (32):

$$\langle p^2 \rangle = -6\pi \left[\frac{f''(r)}{r} - \frac{2f'(r)}{r^2} + \frac{2f(r)}{r^3} \right]_{r=0} \tag{33}$$

Employing L'Hospital's rule one obtains:

$$\langle p^2 \rangle = -2\pi f'''(r)|_{r=0} = \frac{3}{5} \int k_f^2 \rho(r_1) \cdot 4\pi r_1^2 dr_1 + \frac{1}{4} \int \frac{\rho'^2(r)}{\rho(r)} 4\pi r_1^2 dr_1. \tag{34}$$

In the LDA model, (34) with $k_f = [3\pi^2 \rho(r)]^{1/3}$ simplifies to

$$\langle p^2 \rangle = 2(T_0[\rho] + T_w[\rho]). \tag{35}$$

The above solution (35) is identical to the full Thomas-Fermi and Weizsacker components (Murphy 1979). This result is in conformity with the functional forms for kinetic energy for the LDA model (Gunnarsson *et al* 1976, 1977; Alonso and Girifalco 1977, 1978; Deb and Ghosh 1983; Ludenã 1983a, b). The NLDA model, where $k = [3\pi^2 \tilde{\rho}(r_1)]^{1/3}$ for which the $\langle p^2 \rangle$-value is:

$$\langle p^2 \rangle = 2 \left\{ T_w[\rho] + \frac{3}{10} (3\pi^2)^{2/3} \int \tilde{\rho}^{2/3}(r_1) \rho(r_1) 4\pi r_1^2 dr \right\}. \tag{36}$$

Another approximation, viz., $k_f = [3\pi^2 \rho(|\mathbf{r}_1 - \mathbf{r}_2|)]$ was also tried out which leads to a gross overestimate of the $\langle p^2 \rangle$-value

$$\langle p^2 \rangle = 2\{T_w[\rho] + \frac{3}{10} (3\pi^2)^{2/3} \rho^{2/3}(0) N\}. \tag{37}$$

In the LDA model, the full Thomas-Fermi and Weizsacker contributions to kinetic energy are unacceptable features. As is known from numerous numerical and theoretical studies (Murphy 1979), the total kinetic energy may be represented fully by one term (e.g. T_0) and a fraction of the other one (e.g. $1/9\, T_w$) as the correction term. However, from these analyses, the NLDA model seems to yield a much more reasonable value for the kinetic energy (Gunnarsson *et al* 1976, 1977; Alonso and Girifalco 1977, 1978; Deb and Ghosh 1983; Ludeña 1983a, b).

In the next section the results for the Compton profile, $J(q)$ for the nitrogen and argon atoms employing the NLDA model are presented.

4. Results and discussion

The $\tilde{\rho}(r)$ for nitrogen and argon atoms were evaluated via (28) by a Regula-Falsi method. It may be noted that $\tilde{\rho}(0)$ is not zero for any atom with more than two electrons

contrary to Deb and Ghosh (1983), where $\tilde{\rho}(r)/(\rho(r)$ was determined to be zero numerically at $r = 0$. This can be easily verified from (25). For atoms with two electrons, $\tilde{\rho}(r) = 0$ for all r is a particular solution in which case

$$\Gamma(\mathbf{r}/\mathbf{r}') = \rho^{1/2}(\mathbf{r})\rho^{1/2}(\mathbf{r}'), \tag{38}$$

and employing (8)

$$\gamma(\mathbf{p}) = (FT\rho^{1/2})^2. \tag{39}$$

The $B(r)$ was computed from (24) and then the Compton profile was extracted via the relation

$$J(q) = \frac{1}{\pi}\int B(r)\cos(qr)\,dr. \tag{40}$$

The results for $J(q)$ for nitrogen and argon atoms are presented in table 1. It may be seen that the overall prediction of $J(q)$ is indeed a good one. The $J(0)$ value which is numerically equal to half the $\langle p^{-1}\rangle$-value seems to be estimated extremely well, the typical relative percent error being less than one percent.

5. Concluding remarks

The present work reports for the first time a reasonably accurate method for extracting atomic Compton profiles exclusively from the knowledge of electron density. This vital link is established via the reciprocal form factor. Also, a better and a more direct

Table 1. A comparison of Compton profiles for nitrogen and argon atoms employing the NLDA model and the NHF wavefunctions (all values are in Hartree atomic units).

	Nitrogen		Argon	
q	NLDA[a,b]	NHF[c]	NLDA[a,b]	NHF[c]
0	2·7560	2·7986	5·0468	5·0635
0·05486	2·7471	2·7910	5·0325	5·0563
0·13960	2·6990	2·7498	4·9557	5·0156
0·21672	2·6223	2·6819	4·8336	4·9438
0·57765	2·0169	2·0615	3·8758	4·1092
0·92748	1·3949	1·3372	2·8809	2·8925
1·4672	0·7847	0·6430	1·9015	1·5935
2·2768	0·3236	0·2953	1·0751	0·9516
6·0657	0·0261	0·0450	0·2390	0·2433

[a] The electron density $\rho(r)$ was computed from Near Hartree Fock wavefunctions (NHF) of Clementi E and Roetti C (1974) *At. Data and Nucl. Data Tables* **14** 177.
[b] The present work employing the non local density approximation. See text for details.
[c] The $J(q)$ for the NHF framework was extracted via direct Fourier transformation of NHF wavefunctions.

method for determination of $\tilde{\rho}(r)$ is made possible with an assumption of spherical symmetry of $\rho(r)$ for atoms.

The present procedure is unsurpassed in accuracy in estimation of the Compton profiles by all currently known methods viz. the BKCM, Lam and Platzman 1974, and Gadre and Chakravorty (1986) procedures. The present work is particularly relevant in the light of recent developments in the density functional theory (see for example, Bamzai and Deb 1981; Parr 1983) since an explicit transformation between ρ and γ is as yet unknown. An extension to molecules (Pathak *et al* 1984) would be interesting though far from straightforward.

Thus, the reciprocal form factor provides an useful connection between electron density and Compton profile for atoms.

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