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Toshikatsu Koga

Department of Applied Chemistry and Department of Applied Science for Energy, Muroran Institute of Technology, Muroran, Hokkaido, 050 Japan
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Rigorous relations between the moments $\langle p_x^l p_y^m p_z^n \rangle$ and $\langle p^n \rangle$ and the characteristic function $B(r)$ of the momentum density distribution $\rho(p)$ are here generalized to the case of negative l , m , and n . A simple application is given which illustrates that the present results enable us to obtain the moments of momenta without referring to any momentum-space quantity.

I. INTRODUCTION

The characteristic function $B(r) [= \int d\mathbf{p} \exp(-i\mathbf{p}r) \rho(\mathbf{p})]$ of the electron momentum density $\rho(\mathbf{p})$ is used to facilitate the analysis of experimental Compton profiles¹ and its fundamental properties have been discussed in detail by Weyrich *et al.*² and Thakkar *et al.*³ In a previous paper,⁴ we have shown that $B(r)$ and its spherical average

$$b(r) \left[= (4\pi)^{-1} \int_0^{2\pi} d\phi \int_0^\pi \sin \theta B(r) \right]$$

are useful for the calculation of the moments $\langle p_x^l p_y^m p_z^n \rangle$ and $\langle p^n \rangle$ where $p = |\mathbf{p}| = (p_x^2 + p_y^2 + p_z^2)^{1/2}$. The resultant relations are

$$\begin{aligned} \langle p_x^l p_y^m p_z^n \rangle &= i^{l+m+n} B^{(l,m,n)}(0), \\ \langle p^n \rangle &= \begin{cases} (-1)^{3n/2} (n+1) b^{(n)}(0) & \text{for even } n, \\ (-1)^{(n+1)/2} [2(n+1)/\pi] \int_0^\infty dr r^{-1} b^{(n)}(r) & \text{for odd } n, \end{cases} \end{aligned} \quad (1)$$

where $B^{(l,m,n)}(r)$ and $b^{(n)}(r)$ denote, respectively, $\partial^{l+m+n} B(r) / \partial x^l \partial y^m \partial z^n$ and $d^n b(r) / dr^n$, and l , m , and n are nonnegative integers.

In this paper, we discuss the corresponding formulas for negative integers l , m , and n , in order to complete a general relation between the characteristic function and the moments of momenta. The results are illustrated by the calculation of the moments $\langle p^n \rangle$ for several Slater-type orbitals.

II. $B(r)$ AND $\langle p_x^{-l} p_y^{-m} p_z^{-n} \rangle$

We assume l , m , and n are positive integers. By definition,

$$\begin{aligned} \langle p_x^{-l} p_y^{-m} p_z^{-n} \rangle &= \int d\mathbf{p} p_x^{-l} p_y^{-m} p_z^{-n} \rho(\mathbf{p}) \\ &= (2\pi)^{-3} \int d\mathbf{r} B(r) \left[\int d\mathbf{p} p_x^{-l} p_y^{-m} p_z^{-n} \exp(+i\mathbf{p}r) \right]. \end{aligned} \quad (3)$$

Since the Fourier transform of p_x^{-l} is $i^l \text{sgn}(x)(\pi/2)^{1/2} \times [(l-1)!]^{-1} x^{l-1}$ (Ref. 5), Eq. (3) is rewritten as

$$\begin{aligned} \langle p_x^{-l} p_y^{-m} p_z^{-n} \rangle &= 2^{-3} i^{l+m+n} [(l-1)! (m-1)! (n-1)!]^{-1} \\ &\times \int d\mathbf{r} B(r) [\text{sgn}(x) x^{l-1} [\text{sgn}(y) y^{m-1} [\text{sgn}(z) z^{n-1}]]. \end{aligned} \quad (4)$$

It is then clear that $\langle p_x^{-l} p_y^{-m} p_z^{-n} \rangle$ vanishes if one of l , m , and n is odd, because $B(r)$ is an even function. For even l , m , and n , we finally obtain

$$\begin{aligned} \langle p_x^{-l} p_y^{-m} p_z^{-n} \rangle &= i^{l+m+n} [(l-1)! (m-1)! (n-1)!]^{-1} \\ &\times \int_0^\infty \int_0^\infty \int_0^\infty dx dy dz x^{l-1} y^{m-1} z^{n-1} B(r). \end{aligned} \quad (5)$$

When only one or two components are concerned, Eq. (5) is reduced to

$$\langle p_x^{-l} \rangle = i^l [(l-1)!]^{-1} \int_0^\infty dx x^{l-1} B(x, 0, 0), \quad (6a)$$

$$\begin{aligned} \langle p_x^{-l} p_y^{-m} \rangle &= i^{l+m} [(l-1)! (m-1)!]^{-1} \\ &\times \int_0^\infty \int_0^\infty dx dy x^{l-1} y^{m-1} B(x, y, 0), \end{aligned} \quad (6b)$$

and their analogs.

When positive and negative l , m , and n are mixed, equations with mixed form of Eqs. (1) and (5) are obtained. For example,

$$\begin{aligned} \langle p_x^{+l} p_y^{-m} p_z^{-n} \rangle &= i^{-l+m+n} [(m-1)! (n-1)!]^{-1} \\ &\times \int_0^\infty \int_0^\infty dy dz y^{m-1} z^{n-1} B^{(l,0,0)}(0, y, z), \end{aligned} \quad (7a)$$

$$\langle p_x^{+l} p_y^{+m} p_z^{-n} \rangle = i^{-l-m+n} [(n-1)!]^{-1} \int_0^\infty dz z^{n-1} B^{(l,m,0)}(0, 0, z), \quad (7b)$$

where all of l , m , and n are assumed to be even.

III. $b(r)$ AND $\langle p^{-n} \rangle$

Since $b(r)$ is related to the radial momentum density

$$I(p) \left[= \int_0^{2\pi} d\phi_p \int_0^\pi \sin \theta_p p^2 \rho(p) \right]$$

through

$$rb(r) = \int_0^\infty dp \sin(pr) [I(p)/p],$$

$$\begin{aligned} \langle p^{-n} \rangle &= \int_0^\infty dp p^{-n} I(p) \\ &= (2/\pi) \int_0^\infty dr r b(r) \left[\int_0^\infty dp p^{n-1} \sin(pr) \right]. \end{aligned} \quad (8)$$

For a special case of $n=1$, we obtain

$$\langle p^{-1} \rangle = (2/\pi) \int_0^\infty dr b(r), \quad (9)$$

since $\int_0^\infty dp \sin(pr) = 1/r$ in the sense of hyperfunctions.⁶ For $n \geq 2$, the integral in the square brackets of Eq. (8) is a special case of a more general integral $\int_0^\infty dp \sin(pr)/p^a$ ($a, r > 0$). By taking its finite part (*partie finie*), the latter integral is found to be⁷

TABLE I. Existing moments $\langle p^n \rangle$ for the first six Slater-type orbitals with exponent ζ .

Orbital	$\langle p^n \rangle / \zeta^n$														
	$n = -6$	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8
1s	...	...	...	...	5	$\frac{16}{3\pi}$	1	$\frac{8}{3\pi}$	1	$\frac{16}{3\pi}$	5	...	...	...	...
2s	...	...	...	...	11	$\frac{368}{45\pi}$	1	$\frac{8}{5\pi}$	$\frac{1}{3}$	$\frac{16}{15\pi}$	1	...	...	...	...
2p	...	...	21	$\frac{256}{15\pi}$	$\frac{7}{3}$	$\frac{64}{15\pi}$	1	$\frac{128}{45\pi}$	1	$\frac{64}{15\pi}$	$\frac{7}{3}$	$\frac{256}{15\pi}$	21	...	...
3s	...	...	...	...	$\frac{93}{5}$	$\frac{5632}{525\pi}$	1	$\frac{128}{105\pi}$	$\frac{1}{5}$	$\frac{256}{525\pi}$	$\frac{1}{5}$	$\frac{128}{105\pi}$	1	$\frac{5632}{525\pi}$	$\frac{93}{5}$
3p	...	...	$\frac{289}{5}$	$\frac{6656}{175\pi}$	$\frac{37}{9}$	$\frac{9088}{1575\pi}$	1	$\frac{9472}{4725\pi}$	$\frac{7}{15}$	$\frac{128}{105\pi}$	$\frac{17}{45}$	$\frac{512}{315\pi}$	$\frac{9}{5}$	...	...
3d	$\frac{429}{5}$	$\frac{2048}{35\pi}$	$\frac{33}{5}$	$\frac{1024}{105\pi}$	$\frac{9}{5}$	$\frac{2048}{525\pi}$	1	$\frac{512}{175\pi}$	1	$\frac{2048}{525\pi}$	$\frac{9}{5}$	$\frac{1024}{105\pi}$	$\frac{33}{5}$	$\frac{2048}{35\pi}$	$\frac{429}{5}$

$$\int_0^\infty dp \sin(pr)/p^a = \begin{cases} \pi r^{a-1} / [2\Gamma(a) \sin(\pi a/2)] & \text{for } a \neq \text{even integer,} \\ (-1)^{a/2} r^{a-1} [(a-1)!]^{-1} [\ln(r) - \psi(a)] & \text{for } a = \text{even integer,} \end{cases} \quad (10)$$

where $\psi(a) = -\gamma + \sum_{n=1}^\infty (a-1)/[n(a-1+n)]$ is the digamma function with γ being the Euler constant. We therefore obtain

$$\langle p^{-n} \rangle = \begin{cases} (-1)^{n/2-1} [(n-2)!]^{-1} \int_0^\infty dr r^{n-1} b(r) & \text{for even } n, \\ (-1)^{(n-1)/2} (2/\pi) [(n-2)!]^{-1} \int_0^\infty dr r^{n-1} b(r) [\ln(r) - \psi(n-1)] & \text{for odd } n. \end{cases} \quad (11)$$

Note that for a positive integer n , $\psi(n)$ is simplified to the finite sum $-\gamma + 1 + 1/2 + 1/3 + \dots + 1/(n-1)$. The results for $\langle p^{-1} \rangle$ and $\langle p^{-2} \rangle$ agree with those given by Thakkar *et al.*³

IV. A SIMPLE APPLICATION

An important aspect of the characteristic function $B(\mathbf{r})$ is that for one-electron orbitals (e.g., independent-particle model and natural orbital expansion), $B(\mathbf{r})$ is equivalent to the overlap integral $S(\mathbf{r})$.² Therefore we can evaluate the moments $\langle p_x^{+1} p_y^{+m} p_z^{+n} \rangle$ and $\langle p^{+n} \rangle$ directly in position space based on the table of overlap integrals (see, e.g., Refs. 8-10) without invoking the momentum-space concepts such as momentum density (cf. Ref. 11). As a simple application of this method, we have examined the moments $\langle p^{+n} \rangle$ for the first six Slater-type orbitals with exponent ζ . The $b(r)$ functions are obtained as

$$b_{1s}(r) = S_{1s} = \exp(-t)(1+t+t^2/3),$$

$$b_{2s}(r) = S_{2s} = \exp(-t)(1+t+4t^2/9+t^3/9+t^4/45),$$

$$b_{2p}(r) = \frac{1}{3}S_{2p\sigma} + \frac{2}{3}S_{2p\pi} = \exp(-t)(1+t+t^2/3-t^4/45),$$

$$b_{3s}(r) = S_{3s} = \exp(-t)(1+t+7t^2/15+2t^3/15+2t^4/75+t^5/225+t^6/1575),$$

$$b_{3p}(r) = \frac{1}{3}S_{3p\sigma} + \frac{2}{3}S_{3p\pi} = \exp(-t)(1+t+19t^2/45+4t^3/45+4t^4/675-t^5/675-t^6/1575),$$

$$b_{3d}(r) = \frac{1}{5}S_{3d\sigma} + \frac{2}{5}S_{3d\pi} + \frac{2}{5}S_{3d\delta} = \exp(-t)(1+t+t^2/3-2t^4/75-t^5/225+t^6/1575),$$

where $t = \zeta r$. Then applying Eqs. (2) and (11), we have calculated $\langle p^{+n} \rangle$ for various n . The existing moments are summarized in Table I, which of course agree with the results from the momentum-space calculation. Interestingly, we see some regularity for the coefficients $\langle p^n \rangle / \zeta^n$. For 1s, 2p, and 3d orbitals, the coefficients are symmetric with respect to $n=1$, and for 3s orbital they are symmetric with respect to $n=3$. However, there seems to be no regularity for the 2s and 3p orbitals.

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