Functionals of Gegenbauer polynomials and $D$-dimensional hydrogenic momentum expectation values

W. Van Assche
Departement Wiskunde, Katholieke Universiteit Leuven, Celestijnenlaan 200B, B-3001 Heverlee, Belgium

R. J. Yáñez
Departamento de Matemática Aplicada and Instituto Carlos I de Física Teórica y Computacional, Universidad de Granada, 18071 Granada, Spain

R. González-Férez and Jesús S. Dehesa
Departamento de Física Moderna and Instituto Carlos I de Física Teórica y Computacional, Universidad de Granada, 18071 Granada, Spain

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The system of Gegenbauer or ultraspherical polynomials $C_n^\lambda(x); n = 0,1,\ldots$ is a classical family of polynomials orthogonal with respect to the weight function $\omega_\lambda(x) = (1 - x^2)^{\lambda - 1/2}$ on the support interval $[-1,1]$. Integral functionals of Gegenbauer polynomials with integrand $f(x)[C_n^\lambda(x)]^2 \omega_\lambda(x)$, where $f(x)$ is an arbitrary function which does not depend on $n$ or $\lambda$, are considered in this paper. First, a general recursion formula for these functionals is obtained. Then, the explicit expression for some specific functionals of this type is found in a closed and compact form; namely, for the functionals with $f(x)$ equal to $(1 - x^2)^a (1 + x^2)^b$, $\log(1 - x^2)$, and $(1 + x)\log(1 + x)$, which appear in numerous physico-mathematical problems. Finally, these functionals are used in the explicit evaluation of the momentum expectation values $\langle p^a \rangle$ and $\langle \log p \rangle$ of the $D$-dimensional hydrogenic atom with nuclear charge $Z \geq 1$. The power expectation values $\langle p^a \rangle$ are given by means of a terminating $\,_{2}F_{4}$ hypergeometric function with unit argument, which is a considerable improvement with respect to Hey’s expression (the only one existing up to now) which requires a double sum. © 2000 American Institute of Physics.

I. INTRODUCTION

The Gegenbauer polynomials $\{C_n^\lambda(x); n = 0,1,\ldots\}$ form a system of polynomials orthogonal with respect to the weight function

$$\omega_\lambda(x) = (1 - x^2)^{\lambda - 1/2}$$
on the interval $[-1,1]$. They have received a great deal of attention for both fundamental and applied reasons. This is because they naturally appear in the description of numerous mathematical notions (e.g., Legendre functions, spherical and hyperspherical harmonics) and physical phenomena. To mention some, let us point out that the Gegenbauer polynomials are involved in the angular or spatial part of the wave function of physical systems in a central potential in both position and momentum spaces, and in the radial part of the wave function of hydrogenic systems in momentum space, as well as in the eigenfunctions of numerous quantum-mechanical prototypic and effective potentials as, for example, the relativistic harmonic oscillator, the
Demkov–Ostrovsky potentials, and some model molecular potentials, first introduced in the study of spatially confined simple quantum systems and then used to interpret spectra of luminescence centers in some solids.

So, the explicit evaluation of numerous physical quantities, which are described by the expectation values of the corresponding Hermitian operators, necessarily requires the calculation of functionals of Gegenbauer polynomials. In particular, this is the case for quantities like the Boltzmann–Shannon information entropy of single particle systems in a central potential and the radial momentum expectation values and (log p), which are described later. These quantities require the evaluation of the following integrals of squares of Gegenbauer polynomials:

\[ \mathcal{F}_n^\lambda((1-x)^\alpha(1+x)^\beta)) = \int_{-1}^{+1} (1-x)^\alpha (1+x)^\beta [C_n^\lambda(x)]^2 \omega_\lambda(x) dx, \]  
\[ \mathcal{F}_n^\lambda(\log(1-x^2)) = \int_{-1}^{+1} \log(1-x^2) [C_n^\lambda(x)]^2 \omega_\lambda(x) dx, \]  
and

\[ \mathcal{F}_n^\lambda((1+x)\log(1+x)) = \int_{-1}^{+1} (1+x)\log(1+x) [C_n^\lambda(x)]^2 \omega_\lambda(x) dx. \]

These three integrals are particular cases of the following general class of Gegenbauer functionals:

\[ \mathcal{F}_n^\lambda(f(x)) = \int_{-1}^{+1} f(x) [C_n^\lambda(x)]^2 \omega_\lambda(x) dx, \]

where \( f(x) \) is some function which does not depend on \( n \) and \( \lambda \).

This paper has a threefold aim. First, the recursive determination of the general Gegenbauer functional \( \mathcal{F}_n^\lambda(f(x)) \), which is done in Sec. II. Second, the explicit evaluation of the three specific Gegenbauer functionals mentioned previously, which is given in Sec. III. Finally, these explicit expressions are used in Sec. IV to determine the momentum expectation values \( \langle p^a \rangle \), \( a \in \mathbb{R} \), and \( \langle \log p \rangle \) of \( D \)-dimensional hydrogenic systems, which illustrates the usefulness of the aforementioned functionals. The calculation of these momentum quantities is important not only for its own but also because (i) the momentum probability density \( \gamma(p) \) for real \( (D = 3) \) atomic systems has been experimentally measured, and the expectation values themselves can be extracted from the isotropic Compton profiles. Indeed, contrary to the radial expectation values \( \langle r^a \rangle \) for which various analytical formulas in the hydrogenic case are known, there exists only an analytical expression (to the best of our information) for the momentum expectation values \( \langle p^a \rangle \) with integer \( \alpha \) due to Hey. This expression is given by means of a double sum of a rational function with several gamma functions of involved arguments which depend on the two summation indices and the main quantum numbers \( (n,l) \) of the state under consideration. Here, in this paper, the quantities \( \langle p^a \rangle \) with real \( \alpha \) are given by means of a terminating \( _2F_1 \) function with unit argument; thus requiring a single sum.

II. GENERAL GEGENBAUER FUNCTIONALS: A RECURSION FORMULA

The main result of this section is the following

**Theorem 1:** The Gegenbauer functionals

\[ \mathcal{F}_n^\lambda(f(x)) = \int_{-1}^{+1} (1-x^2)^{\lambda-1/2} [C_n^\lambda(x)]^2 f(x) dx, \]

satisfy the recursion relation
\[
\left(\frac{n}{2\lambda}\right)^2 F_n^\lambda(f) - \left(\frac{n+2\lambda-1}{2\lambda}\right)^2 F^\lambda_{n-1}(f) = F^\lambda_{n-2}(f) - F^\lambda_{n-1}(f).
\]  

(3)

**Proof:** In Ref. 21 the following recursive formula for squares of Gegenbauer polynomials is found:

\[
\left(\frac{n}{2\lambda}\right)^2 [C_n^\lambda(x)]^2 = \sum_{k=0}^{n-1} \frac{\lambda+k}{\lambda} [C_k^\lambda(x)]^2 - (1-x^2)[C_{n-1}^\lambda(x)]^2.
\]  

(4)

Multiplying both sides by \((1-x^2)^{\lambda-1/2}f(x)\) and integrating, we obtain

\[
\left(\frac{n}{2\lambda}\right)^2 F_n^\lambda(f) = \sum_{k=0}^{n-1} \frac{\lambda+k}{\lambda} F_k^\lambda(f) - F_{n-1}^\lambda(f),
\]  

(5)

which gives a linear recurrence in \(n\) and \(\lambda\) for \(F_n^\lambda(f)\). Taking (5) for \(n\) and subtracting the same equation for \(n-1\),

\[
\left(\frac{n}{2\lambda}\right)^2 F_n^\lambda(f) - \left(\frac{n-1}{2\lambda}\right)^2 F_{n-1}^\lambda(f) = \frac{n-1+\lambda}{\lambda} F_{n-1}^\lambda(f) + F_{n-2}^\lambda(f) - F_{n-1}^\lambda(f),
\]  

which, after collecting terms, gives

\[
\left(\frac{n}{2\lambda}\right)^2 F_n^\lambda(f) - \left(\frac{n+2\lambda-1}{2\lambda}\right)^2 F_{n-1}^\lambda(f) = F_{n-2}^\lambda(f) - F_{n-1}^\lambda(f).
\]  

(6)

This is a recurrence relation of finite order connecting four "contiguous" \(F_n^\lambda(f)\). If \(F_n^\lambda(1,0)\) is known for \(k=0,1,\ldots,n\), then this allows the computation of \(F_n^\lambda(f)\).

III. SOME GEGENBAUER FUNCTIONALS: EXPLICIT EXPRESSIONS

In this section we obtain closed formula for some specific functionals of Gegenbauer polynomials of the form \(F_n^\lambda(f)\); namely, when

\[f(x) = (1-x)^{\alpha}(1+x)^{\beta}, \quad \log(1-x^2), \quad \text{and} \quad (1+x) \log(1+x).
\]

The corresponding results are given by Theorems 2, 3, and 4, respectively. An important lemma, necessary for the proof of Theorem 4, is also described. This lemma allows us to find the value of another Gegenbauer functional with kernel \(\log(1+x)C_{n-1}^\lambda(x)C_n^\beta(x)\).

**Theorem 2:** The Gegenbauer functionals \(F_n^\lambda(\alpha,\beta) = F_n^\lambda(1-x)^{\alpha}(1+x)^{\beta}\) defined as

\[
F_n^\lambda(\alpha,\beta) = \int_{-1}^{1} (1-x^2)^{\lambda-1/2}[C_n^\lambda(x)]^2(1-x)^\alpha(1+x)^\beta dx
\]  

(7)

have the following values:

\[
F_n^\lambda(\alpha,\beta) = \frac{\sqrt{\pi}\Gamma(\lambda+\alpha+\frac{1}{2})\Gamma(\lambda+\beta+\frac{1}{2})}{\Gamma\left(\frac{\alpha+\beta+1}{2}\right)\Gamma\left(\frac{\alpha+\beta+1}{2}+1\right)} \left(\frac{2\lambda}{n}\right)^2
\times 2F_2\left(-n,n+2\lambda,\lambda+\alpha+\frac{1}{2},\lambda+\beta+\frac{1}{2};\frac{1}{2\lambda+\frac{1}{2}+\alpha+\frac{1}{2},\lambda+\beta+\frac{1}{2}+\alpha+\frac{1}{2}+1}\right).
\]  

(8)
Proof: The Gegenbauer polynomial has the hypergeometric representation

\[ C_n^\lambda(x) = \frac{(2\lambda)_n}{n!} \, _2F_1\left(\frac{-n, n + 2\lambda}{\lambda + \frac{1}{2}}; \frac{1-x}{2}\right). \]

If we use a quadratic transformation formula [Ref. 22, Eq. (9.133) on p. 1070] then this gives

\[ C_n^\lambda(x) = \frac{(2\lambda)_n}{n!} \, _2F_1\left(-\frac{n/2, n/2 + \lambda}{\lambda + \frac{1}{2}}; 1-x^2\right). \]

Observe that for \( n \) even this is a terminating hypergeometric series, but for \( n \) odd this is nonterminating. Now apply the Clausen’s formula [Refs. 1, 23, Eq. (2.5.7) on p. 75] to find

\[ [C_n^\lambda(x)]^2 = \left(\frac{(2\lambda)_n}{n!}\right)^2 \, _3F_2\left(-\frac{n, n + 2\lambda, \lambda}{2\lambda, \lambda + \frac{1}{2}}; 1-x^2\right), \]

which is now always a terminating series. Using this in (7), gives

\[ \mathcal{F}_n^\lambda(\alpha, \beta) = \left(\frac{(2\lambda)_n}{n!}\right)^2 \sum_{k=0}^{n} \frac{(-n)_k(n+2\lambda)_k(\lambda)_k}{(2\lambda)_k(\lambda + \frac{1}{2})_k} \Gamma(\lambda + k + \alpha + \frac{1}{2})\Gamma(\lambda + k + \beta + \frac{1}{2}) \frac{\Gamma(\lambda + k + \alpha + \beta + 1)}{\Gamma\left(\lambda + k + \frac{\alpha + \beta}{2} + 1\right)^2}. \]

The last integral can be evaluated in term of gamma functions, giving

\[ \int_{-1}^{1} (1-x)^{\lambda-1/2+k+a}(1+x)^{\lambda-1/2+k+b}dx = \frac{2^{2\lambda+2k+a+b}\Gamma(\lambda+k+a+\frac{1}{2})\Gamma(\lambda+k+b+\frac{1}{2})}{\Gamma(2\lambda+2k+a+b+1)} \]

\[ = \frac{\sqrt{\pi} \Gamma(\lambda+k+a+\frac{1}{2})\Gamma(\lambda+k+b+\frac{1}{2})}{\Gamma\left(\lambda + k + \frac{\alpha + \beta}{2} + 1\right)^2}. \]

where the last equality follows from the duplication formula for the gamma function. Hence,

\[ \mathcal{F}_n^\lambda(\alpha, \beta) = \frac{\sqrt{\pi} \Gamma(\lambda + \alpha + \frac{1}{2})\Gamma(\lambda + \beta + \frac{1}{2})}{\Gamma\left(\lambda + \frac{\alpha + \beta + 1}{2}\right)^2 \Gamma\left(\lambda + \frac{\alpha + \beta}{2} + 1\right)^2} \times \sum_{k=0}^{n} \frac{(-n)_k(n+2\lambda)_k(\lambda)_k(\lambda + \alpha + \frac{1}{2})_k(\lambda + \beta + \frac{1}{2})_k}{(2\lambda)_k(\lambda + \frac{1}{2})_k(\lambda + \alpha + \frac{1}{2})_k(\lambda + \beta + \frac{1}{2})_k} k! \]

giving the desired result (8).

When \( \alpha = \beta \) then the hypergeometric function simplifies to

\[ \mathcal{F}_n^\lambda(\alpha, \alpha) = \frac{\sqrt{\pi} \Gamma(\lambda + \alpha + \frac{1}{2})}{\Gamma(\lambda + \alpha + 1)} \left(\frac{(2\lambda)_n}{n!}\right)^2 \, _4F_3\left(-\frac{n, n + 2\lambda, \lambda, \lambda + \alpha + \frac{1}{2}}{2\lambda, \lambda + \frac{1}{2}, \lambda + \alpha + \frac{1}{2}}; 1\right). \]

Another simplification occurs when one of the parameters is zero,
Another interesting case occurs when \( \beta = 1 - \alpha \),

\[
\mathcal{F}_n^\lambda(0,\beta) = \frac{\sqrt{\pi} \Gamma(\lambda + \frac{1}{2}) \Gamma(\lambda + \beta + \frac{1}{2})}{\Gamma\left(\lambda + \frac{1}{2}\right) \Gamma\left(\lambda + \beta + 1\right)} \left(\frac{(2\lambda_n)^2}{n!}\right) \times {}_4F_3\left(-n, n + 2\lambda, \lambda, \lambda + \beta + \frac{1}{2}; 2\lambda, \lambda + 1, \lambda + 1; 1\right).
\]

(10)

Theorem 3: The Gegenbauer functional \( J(n, \lambda) = \mathcal{F}_n^\lambda(\log(1 - x^2)) \) defined by

\[
J(n, \lambda) = \int_{-1}^{1} (1 - x^2)^{\lambda - \frac{1}{2}} [C_n^\lambda(x)]^2 \log(1 - x^2) \, dx,
\]

has the expression

\[
J(n, \lambda) = \frac{\Gamma(2\lambda + n) 2^{-2\lambda}}{n! \Gamma^2(\lambda)} \left[ \frac{2\psi(2\lambda + n) - 2\psi(\lambda + n) - 2 \log 2 - \frac{1}{\lambda + n}}{\lambda + n} \right].
\]

Proof: Use

\[
-\frac{2\lambda}{(2\lambda + n)n} \left[ (1 - x^2)^{\lambda + \frac{1}{2}} C_{n-1}^{\lambda+1}(x) \right]' = (1 - x^2)^{\lambda - \frac{1}{2}} C_n^\lambda(x),
\]

then integration by parts gives

\[
J(n, \lambda) = \frac{2\lambda}{(2\lambda + n)n} \int_{-1}^{1} (1 - x^2)^{\lambda + \frac{1}{2}} C_{n-1}^{\lambda+1}(x) [C_n^\lambda(x) \log(1 - x^2)]' \, dx.
\]

Now use \([ C_n^\lambda(x) ]' = 2\lambda C_{n-1}^{\lambda+1}(x)\) to find

\[
J(n, \lambda) = \frac{4\lambda^2}{(2\lambda + n)n} J(n - 1, \lambda + 1) - \frac{2\lambda}{(2\lambda + n)n} \int_{-1}^{1} (1 - x^2)^{\lambda - \frac{1}{2}} 2x C_{n-1}^{\lambda+1}(x) C_n^\lambda(x) \, dx.
\]

Since \( 2x C_{n-1}^{\lambda+1}(x) = (n/\lambda) C_n^\lambda(x) \) + lower degree terms, this gives by orthogonality

\[
J(n, \lambda) = \frac{4\lambda^2}{(2\lambda + n)n} J(n - 1, \lambda + 1) - \frac{2\lambda}{(2\lambda + n)n} \int_{-1}^{1} (1 - x^2)^{\lambda - \frac{1}{2}} [C_n^\lambda(x)]^2 \, dx
\]

\[
= \frac{4\lambda^2}{(2\lambda + n)n} J(n - 1, \lambda + 1) - \frac{\pi 2^{2-2\lambda} \Gamma(n + 2\lambda)}{(2\lambda + n)^{1/2} \Gamma(n + \lambda)n^2}.
\]

Define

\[
K(n, \lambda) = \frac{n! \Gamma^2(\lambda) 2^{2\lambda}}{\Gamma(2\lambda + n)} J(n, \lambda).
\]
then this becomes

\[ K(n, \lambda) = K(n-1, \lambda + 1) - \frac{4\pi}{(2\lambda + n)(n + \lambda)}. \]

This is a nice inhomogeneous recurrence relation. Setting \( B(k) = K(k, \lambda + n - k) \) with \( n \) fixed, gives the first-order recurrence

\[ B(k) = B(k-1) - \frac{4\pi}{(2\lambda + 2n - k)(\lambda + n)}. \]

Solving recursively gives

\[ B(n) = B(0) - \frac{4\pi}{\lambda + n} \sum_{k=1}^{n} \frac{1}{2\lambda + 2n - k}, \]

which in terms of \( K(n, \lambda) \) is

\[ K(n, \lambda) = K(0, \lambda + n) - \frac{4\pi}{\lambda + n} \left[ \psi(2\lambda + 2n) - \psi(2\lambda + n) \right], \]

where \( \psi(x) = \Gamma'(x)/\Gamma(x) \). The initial condition (for \( n = 0 \)) can be checked fairly easy

\[ K(0, \alpha) = \frac{2\pi}{\alpha} \left[ \psi(\alpha + 1/2) - \psi(\alpha + 1) \right], \]

and to finish the proof we need the duplication formula for the psi-function

\[ 2\psi(2z) = 2\log 2 + \psi(z) + \psi(z + 1/2), \]

which applied to \( \psi(2n + 2\lambda) \) leads to the desired expression.

Alternatively one can prove Theorem 3 as follows. Consider the integral

\[ \int_{-1}^{1} (1 - x^2)^{\lambda - 1/2} C_n^\lambda(x)^2 dx = \frac{\pi 2^{1-2\lambda} \Gamma(2\lambda + n)}{n!(\lambda + n)! [\Gamma(\lambda)]^2}, \]

and differentiate this with respect to \( \lambda \). Then this gives the required expression. This method, however, cannot be used for the other functionals.

**Lemma 1:** Let

\[ L(n, \lambda) = \int_{-1}^{1} (1 - x^2)^{\lambda + 1/2} C_n^{\lambda + 1}(x)C_n^\lambda(x) \log(1 + x) dx, \]

then

\[ L(n, \lambda) = \frac{\pi}{n + \lambda} \frac{\Gamma(2\lambda + n + 1)}{\Gamma(\lambda) \Gamma(\lambda + 1) 2^{\lambda}(n-1)!} \left[ \frac{1}{2n + 2\lambda + 1} + \frac{1}{2n + 2\lambda - 1} - \frac{1}{2\lambda + n} \right]. \]

**Proof:** Use

\[ -\frac{2(\lambda + 1)}{(2\lambda + n + 1)(n-1)} \left[ (1 - x^2)^{\lambda + 3/2} C_n^{\lambda + 2}(x) \right]' = (1 - x^2)^{\lambda + 1/2} C_n^{\lambda + 1}(x), \]

which holds for \( n \geq 2 \), then integration by parts gives
\[ L(n, \lambda) = \frac{2\lambda+2}{(2\lambda+n+1)(n-1)} \int_{-1}^{1} (1-x^2)^{\lambda+3/2} C_{n-2}^{\lambda+2}(x) \left[ C_n^{\lambda}(x) \log(1+x) \right]' \, dx. \]

Since \( [C_n^{\lambda}(x)]' = 2\lambda C_{n-1}^{\lambda+1}(x) \), this gives
\[ L(n, \lambda) = \frac{4\lambda(\lambda+1)}{(2\lambda+n+1)(n-1)} L(n-1, \lambda+1) \]
\[ + \frac{2(\lambda+1)}{(2\lambda+n+1)(n-1)} \int_{-1}^{1} (1-x^2)^{\lambda+3/2} C_{n-2}^{\lambda+2}(x) C_n^{\lambda}(x) \frac{dx}{1+x}. \]

(12)

For the last integral we observe that
\[ (1-x^2)^{\lambda+3/2} C_{n-2}^{\lambda+2}(x) C_n^{\lambda}(x)(1+x)^{-1} = (1-x^2)^{\lambda-1/2} C_n^{\lambda}(x)(1-x^2)(1-x) C_{n-2}^{\lambda+2}(x). \]

If we expand the polynomial between square brackets into Gegenbauer polynomials \( C_n^{\lambda}(x) \), then
\[ (1-x^2)(1-x) C_{n-2}^{\lambda+2}(x) = \sum_{k=0}^{n+1} A_k C_k^{\lambda}(x), \]

and we only need to know the coefficient \( A_n \) of \( C_n^{\lambda}(x) \). We can find this coefficient by comparing the coefficients of \( x^n \), and taking into account that
\[ C_n^{\lambda}(x) = \frac{2^n \Gamma(\lambda+n)}{\Gamma(\lambda)n!} x^n + \text{lower order terms}, \]

we thus find
\[ A_n = \frac{2^n \Gamma(\lambda+n)}{\Gamma(\lambda)n!} = -\frac{2^{n-2} \Gamma(\lambda+n)}{\Gamma(\lambda+2)(n-2)!}, \]

so that \( A_n = -n(n-1)/[4\lambda(\lambda+1)] \). Hence
\[ \int_{-1}^{1} (1-x^2)^{\lambda+3/2} C_{n-2}^{\lambda+2}(x) C_n^{\lambda}(x) \frac{dx}{1+x} = -\frac{n(n-1)}{4\lambda(\lambda+1)} \int_{-1}^{1} (1-x^2)^{\lambda-1/2} [C_n^{\lambda}(x)]^2 \, dx \]
\[ = -\frac{n(n-1)}{4\lambda(\lambda+1)} \frac{\pi \Gamma(\lambda+n+2)}{(\lambda+n)!} 2^{-2\lambda+1}. \]

If we insert this in (12) then we find
\[ L(n, \lambda) = \frac{4\lambda(\lambda+1)}{(2\lambda+n+1)(n-1)} L(n-1, \lambda+1) - \frac{\pi 2^{-2\lambda} \Gamma(\lambda+n+2)}{\Gamma(\lambda+1)(n+\lambda)(2\lambda+n+1)(n-1)!}. \]

In order to solve this recurrence relation, we set
\[ M(n, \lambda) = \frac{\Gamma(\lambda) \Gamma(\lambda+1) 2^{2\lambda}(n-1)!}{\Gamma(2\lambda+n+1)} L(n, \lambda), \]

to find
\[ M(n, \lambda) = M(n-1, \lambda+1) - \frac{\pi}{(n+\lambda)(2\lambda+n+1)(2\lambda+n)}. \]
Decreasing \( n \) by one and increasing \( \lambda \) by one successively gives

\[
M(n, \lambda) = M(1, n + \lambda - 1) = \frac{\pi}{n + \lambda} \sum_{k=2}^{n} \frac{1}{(2n + 2\lambda - k + 1)(2n + 2\lambda - k)}.
\]

Decomposition into partial fractions gives

\[
\sum_{k=2}^{n} \frac{1}{(2n + 2\lambda - k + 1)(2n + 2\lambda - k)} = \sum_{k=2}^{n} \left[ \frac{1}{2n + 2\lambda - k} - \frac{1}{2n + 2\lambda - k + 1} \right] = \frac{1}{2\lambda + n} \frac{1}{(2n + 2\lambda - 1)}.
\]

and thus

\[
M(n, \lambda) = M(1, n + \lambda - 1) = \frac{\pi}{n + \lambda} \left[ \frac{1}{2\lambda + n} - \frac{1}{(2n + 2\lambda - 1)} \right].
\]

We only need to compute \( M(1, n + \lambda - 1) \). Observe that

\[
L(1, n + \lambda - 1) = 2(n + \lambda - 1) \int_{-1}^{1} (1 - x^2)^{n + \lambda - 1/2} \log(1 + x) \, dx.
\]

Use

\[
[(1 - x^2)^{n + \lambda + 1/2}]' = -(2n + 2\lambda + 1)x(1 - x^2)^{n + \lambda - 1/2},
\]

then

\[
L(1, n + \lambda - 1) = -\frac{2n + 2\lambda - 2}{2n + 2\lambda + 1} \int_{-1}^{1} \log(1 + x)[(1 - x^2)^{n + \lambda + 1/2}]' \, dx
\]

\[
= \frac{2n + 2\lambda - 2}{2n + 2\lambda + 1} \int_{-1}^{1} (1 - x)^{n + \lambda + 1/2}(1 + x)^{n + \lambda - 1/2} \, dx
\]

\[
= (n + \lambda - 1) 2^{2n + 2\lambda + 1} \frac{\Gamma^2(n + \lambda + 1/2)}{\Gamma(2n + 2\lambda + 2)}.
\]

This gives for \( M(1, n + \lambda - 1) \),

\[
M(1, n + \lambda - 1) = \frac{\pi}{n + \lambda} \frac{1}{2n + 2\lambda + 1},
\]

and thus

\[
M(n, \lambda) = \frac{\pi}{n + \lambda} \left( \frac{1}{2n + 2\lambda + 1} + \frac{1}{2n + 2\lambda - 1} - \frac{1}{2\lambda + n} \right),
\]

from which the lemma follows.

We have now the tools to prove

**Theorem 4:** The Gegenbauer functionals \( I(n, \lambda) = \mathcal{F}_n^\lambda((1+x)\log(1+x)) \) defined as

\[
I(n, \lambda) = \int_{-1}^{1} (1 - x^2)^{\lambda - 1/2} \{ C_n^\lambda(x) \}^2(1 + x)\log(1 + x) \, dx,
\]

(13)
have the following value:

\[ I(n, \lambda) = \frac{\pi \Gamma(2\lambda + n)2^{-2\lambda}}{n! \Gamma^2(\lambda)} \]

\[ \times \left( \frac{2}{n + \lambda} \left[ 1 - \log 2 + \psi(2\lambda + n) - \psi(\lambda + n) \right] - \frac{4(2\lambda - 1)}{4(n + \lambda)^2 - 1} - \frac{1}{(n + \lambda)^2} \right). \]

**Proof:** Use

\[ I \sim_n \frac{2\lambda}{(2\lambda + n)n} \int_{-1}^{1} (1 - x^2)^{\lambda + 1/2} C_{n-1}^{\lambda+1}(x)[C_n^{\lambda}(x)(1 + x)\log(1 + x)]'dx \]

\[ = \frac{4\lambda^2}{(2\lambda + n)n} \int_{-1}^{1} (1 - x^2)^{\lambda + 1/2} [C_{n-1}^{\lambda+1}(x)]^2 (1 + x)\log(1 + x)dx \]

\[ + \int_{-1}^{1} (1 - x^2)^{\lambda + 1/2} C_{n-1}^{\lambda+1}(x)C_n^{\lambda}(x)[1 + \log(1 + x)]dx. \]

Observe that \( C_{n-1}^{\lambda+1}(x)C_n^{\lambda}(x) \) is an odd function, hence

\[ \int_{-1}^{1} (1 - x^2)^{\lambda + 1/2} C_{n-1}^{\lambda+1}(x)C_n^{\lambda}(x)dx = 0, \]

and thus

\[ I(n, \lambda) = \frac{4\lambda^2}{(2\lambda + n)n} I(n-1, \lambda + 1) + \frac{2\lambda}{(2\lambda + n)n} L(n, \lambda), \]

where \( L(n, \lambda) \) is the expression given in the previous lemma. If we set

\[ K(n, \lambda) = \frac{2\lambda \Gamma^2(\lambda)n!}{\Gamma(2\lambda + n)} I(n, \lambda), \]

and if we use the expression for \( L(n, \lambda) \) given in the previous lemma, then we have

\[ K(n, \lambda) = K(n-1, \lambda + 1) + \frac{8\pi}{4(n+\lambda)^2 - 1} - \frac{2\pi}{(n+\lambda)(2\lambda + n)}. \]

Solving recursively gives

\[ K(n, \lambda) = K(0, \lambda + n) + \frac{8\pi n}{4(n+\lambda)^2 - 1} - \frac{2\pi}{n+\lambda} \sum_{k=1}^{n} \frac{1}{2\lambda + 2n - k} \]

\[ = K(0, \lambda + n) + \frac{8\pi n}{4(n+\lambda)^2 - 1} - \frac{2\pi}{n+\lambda} \left[ \psi(2\lambda + 2n) - \psi(2\lambda + n) \right]. \]

So all one still needs is \( K(0, n+\lambda) \). It is not too hard to compute.
and using this in the previous formula then gives the desired result, provided one uses the duplication formula for the gamma function.

Note that, in principle, Theorem 4 can be proved by taking a derivative with respect to $\beta$ in expression (10) and then taking $\beta = 1$.

IV. MOMENTUM EXPECTATION VALUES OF THE D-DIMENSIONAL HYDROGEN ATOM

The momentum expectation values $\langle p^\alpha \rangle$, $\alpha \in \mathbb{R}$, of an $N$-electron system in an arbitrary quantum-mechanical density $\gamma(\vec{p})$, are defined by

$$\langle p^0 \rangle = \int p^0 \gamma(\vec{p}) d\vec{p}. \quad (14)$$

These quantities are physically meaningful and/or experimentally accessible. Let us remember the exact relations

$$\langle p^{-1} \rangle = 2J(0), \quad \langle p^0 \rangle = N,$$

$$\langle p^2 \rangle = 2T_{NR}, \quad \langle p^4 \rangle = -8e^2T_{BP},$$

where $J(0)$, $N$, $T_{NR}$, and $T_{BP}$ are the peak height of the isotropic Compton profile, the number of electrons, the nonrelativistic electron kinetic energy, and the Breit–Pauli mass-velocity correction at first order to the energy, respectively, and $e$ denotes the speed of light. Also the following empirical and highly accurate relationships have been found:

$$\langle p \rangle = -\pi K_0, \quad \langle p^3 \rangle = \frac{3\pi^2}{2} \langle p \rangle$$

and

$$V_{ee} = dN^{43/3} \langle p^3 \rangle^{1/3}; \quad d = 0.135 \pm 0.003,$$

where $K_0$, $\langle p \rangle$, and $V_{ee}$ are the Dirac–Slater exchange energy, the average electron density in position space, and the total electron–electron repulsion energy, respectively. Moreover, the value $\langle p^3 \rangle$ is roughly proportional to the initial value of the Patterson function of x-ray crystallography.

The momentum expectation values $\langle p^\alpha \rangle$ have been recently evaluated for $-2 \leq \alpha \leq 4$ particularly by means of huge numerical Hartree–Fock calculations for all existing neutral atoms and 54 singly charged atomic cations from He$^+$ (atomic number $Z = 2$) to Cs$^+$ ($Z = 55$) and 43 anion from $Z^-$ ($Z = 1$) to $\Gamma^-$ ($Z = 53$) in their experimental ground states. Moreover, some inequalities for various momentum expectation values and other density functionals or even with some local properties of the system have been found either rigorously or semiclassically. Also, analytical approximations for these momentum quantities have been derived in neutral atoms.

However, the exact values of these quantities cannot be found because the atomic wave function is not known except for hydrogenic systems. The purpose of this section is the analytic determination of the momentum expectation values $\langle p^\alpha \rangle$, $\alpha \in \mathbb{R}$, and $\langle \log p \rangle$ of a $D$-dimensional hydrogen atom in an arbitrary quantum-mechanical state. It is known that this system is described by the radially symmetric Coulomb potential
\[
V(r) = -\frac{1}{r}, \quad r^2 = \sum_{i=1}^{D} x_i^2
\]
and its associated Born momentum probability density is
\[
\gamma(\vec{p}) = K_{n,l}^2 \frac{(\eta p)^{2l}}{(1 + \eta^2 p^2)^{D-1+\nu}} \left[ C_{n-l-1}^{l+D-1} \frac{(1 - \eta^2 p^2)}{(1 + \eta^2 p^2)} \right] |Y_{l,\mu}(\Omega_D)|^2, \tag{15}
\]
where \(\eta\) is a parameter which depends on the principal quantum number \(n\) and the dimension \(D\) by
\[
\eta = n + \frac{D - 3}{2}.
\]
\(Y_{l,\mu}(\Omega_D)\) is a hyperspherical harmonic which depends on the orbital quantum number \(l\) and the magnetic quantum numbers \(\mu, z\) and the normalization constant \(K_{n,l}\) is given by
\[
K_{n,l} = \left( \frac{(n-l-1)!}{2\pi(n+l+D-3)!} \right)^{1/2} \frac{2^{2l+D} \Gamma \left( 1 + \frac{D-1}{2} \right) \eta^{(D+1)/2}}{2^{l+D} \Gamma \left( 1 + \frac{D-1}{2} \right)}. \]
Taking the explicit expression (15) for \(\gamma(\vec{p})\) into Eq. (14) together with the use of the orthonormalization condition of the hyperspherical harmonics we find that
\[
\langle p^\alpha \rangle = \frac{K_{n,l}^2}{2^{2l+D+\nu} \eta^{\alpha}} \int_{-1}^{+1} (1-t)^{\nu+(\alpha-1)/2} (1+t)^{\nu-(\alpha-1)/2} (\nu+\alpha+1/2)^{\nu+3-\alpha/2} (\nu+\alpha+1/2)^{-\nu-1/2} \left[ C_k^l(t) \right]^2 dt \tag{16}
\]
with \(k = n - l - 1\) and \(\nu = l + (D-1)/2\). Using (8) we find the closed formula
\[
\langle p^\alpha \rangle = \frac{2^{1-2\nu}\sqrt{\pi}}{k!\eta^\alpha} \frac{(k+\nu)\Gamma(k+2\nu)}{\Gamma^2(\nu+\frac{1}{2})} \frac{\Gamma(\nu+\alpha+1/2)\Gamma(\nu+3-\alpha/2)}{\Gamma(\nu+1)\Gamma(\nu+\alpha+1/2)}
\times \frac{\alpha+1/2}{2\nu, \nu+1/2, \nu+1, \nu+\frac{3}{2}} \tag{17}
\]
which clearly holds for all values of \(\alpha\): \(-2l-D<\alpha<2l+D+2\). The \(F_4\)-hypergeometric function in (17) is terminating (i.e., it is a finite series), Saalschützian (or balanced), i.e., \(1+a_1+a_2+a_3+a_4=b_1+b_2+b_3+b_4\), and with unit argument.\(^{23}\) The lack of a general summation formula for a terminating, Saalschützian \(F_4\)-hypergeometric function with unit argument, does not allow us to obtain a general closed formula for \(\langle p^\alpha \rangle\) for general \(\alpha\). Let us study in detail some special cases.

1. For \(\alpha=0\), we obtain
\[
\langle p^0 \rangle = \frac{2^{1-2\nu}\sqrt{\pi}(k+\nu)\Gamma(k+2\nu)}{\Gamma(\nu+1)\Gamma(\nu+\frac{1}{2})} \frac{\Gamma(\nu+\alpha+1/2)\Gamma(\nu+3-\alpha/2)}{\Gamma(\nu+1)\Gamma(\nu+\alpha+1/2)} \langle F_4(-k,\nu,k+2\nu) \rangle
\]
Using Saalschütz’s theorem\(^{23}\)
\[
\langle F_4(-k,\nu,k+2\nu) \rangle = \frac{(c-a)_n(c-b)_n}{(c)_n(c-a-b)_n}
\]
we obtain
\[
\langle p^0 \rangle = 1
\]
as expected.

(2) For \(\alpha = 2\), the result is
\[
\langle p^2 \rangle = \frac{2^{1-2\nu} \sqrt{\pi} (k + \nu) \Gamma(k + 2\nu)}{\eta^2 \Gamma\left(\nu + \frac{1}{2}\right) \Gamma(\nu + 1)} \ {}_1 F_2 \left(\begin{array}{c}
-k, k + 2\nu \\
2\nu, \nu + 1
\end{array} ; 1\right).
\]
Again, the use of Saalschutz’s theorem, allows us to find
\[
\langle p^2 \rangle = \frac{1}{\eta^2}.
\]
Now, let us calculate the logarithmic expectation value \(\langle \log p \rangle\), which is defined by
\[
\langle \log p \rangle = \int \log p \gamma(\vec{p}) d\vec{p}.
\]
Taking into account the explicit expression (15) for the momentum density \(\gamma(\vec{p})\) we find
\[
\langle \log p \rangle = \frac{K^2}{2^{2
\nu+D+2} \eta^2} \left( -2 \log \eta + I_1 - I_2 \right),
\]
where the symbols \(I_1\) and \(I_2\) denote
\[
I_1 = \int_{-1}^{+1} (1 - t^2)^{\nu-\frac{1}{2}} (1 + t) \log(1 - t) \left[ C^\nu_k(t) \right]^2 dt = J(k, \nu) - I(k, \nu),
\]
\[
I_2 = \int_{-1}^{+1} (1 - t^2)^{\nu-\frac{1}{2}} (1 + t) \log(1 + t) \left[ C^\nu_k(t) \right]^2 dt = I(k, \nu),
\]
respectively, so that
\[
\langle \log p \rangle = \frac{K^2}{2^{2\nu+D+2} \eta^2} \left[ -2 \log \eta + J(k, \nu) - 2I(k, \nu) \right]
\]
with \(k = n - l - 1\) and \(\nu = l + (D - 1)/2\). The use of the values of \(J(k, \nu)\) and \(I(k, \nu)\) supplied by Theorems 3 and 4, respectively, leads us to
\[
\langle \log p \rangle = - \log \eta - 1 + \frac{2(2\nu - 1) \eta}{4 \eta^2 - 1}.
\] (18)

For hydrogenic atoms with nuclear charge \(Z \geq 1\), in which the Coulomb potential is \(-Z/r\), the momentum density is \(Z^{-D} \gamma(\vec{p}/Z)\). The power and logarithmic expectation values, given by Eqs. (17) and (18), respectively, have to be modified in the form \(Z^a \langle p^a \rangle\) and \(\log Z + \langle \log p \rangle\), respectively.

Finally, let us point out that the momentum expectation power and logarithmic values for the ground state of a \(D\)-dimensional hydrogenic atom with nuclear charge \(Z\) are
\[ \langle p^\alpha \rangle = \frac{2^{\alpha/2} \Gamma\left(\frac{D-\alpha}{2} \right) \Gamma\left(\frac{D+\alpha}{2} \right)}{D^{\alpha/2} \Gamma(D/2)} Z^\alpha, \quad -D < \alpha < D+2, \]

and

\[ \langle \log p \rangle = \log \left( \frac{D - 1/2}{Z} \right) - \frac{1}{D}, \]

respectively.

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