EXPECTATION VALUES $\langle r^p \rangle$ FOR HARMONIC OSCILLATOR IN $\mathbb{R}^n$

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Abstract. We evaluate the matrix elements $\langle r^p \rangle$ for the $n$-dimensional harmonic oscillator in terms of the dual Hahn polynomials and derive a corresponding three-term recurrence relation and a Pasternack-type reflection relation. A short review of similar results for nonrelativistic hydrogen atom is also given.

1. An Introduction

The purpose of this note is to present a simple evaluation of the expectation values $\langle r^p \rangle$ for the $n$-dimensional harmonic oscillator in terms of the dual Hahn polynomials by direct integration. Other methods of solving similar problems in elementary quantum mechanics appeal to general principles and involve the Hellmann–Feynman theorem (see [6], [7], [8] and references given there, textbooks [27, 32, 11, 40], commutation relation ([23, 20, 42, 43]), and dynamical groups ([3, 4, 9, 10, 16, 37, 41]). Our approach allows to study these expectation values with the help of the advanced theory of classical polynomials [2], [25], and [35]. We recall also that the first-order of the time-independent perturbation theory equates the energy correction to the expectation value of the perturbing potential. Thus expressions of the form $\langle r^p \rangle$ gain utmost importance.

The plan of the paper is as follows. We review results on expectation values $\langle r^p \rangle$ for the nonrelativistic hydrogenlike wave functions first and then extend them, in a similar fashion, to the case of $n$-dimensional harmonic oscillator. An attempt to collect the available literature is made.

2. Expectation Values $\langle r^p \rangle$ for Coulomb Problems

The problem of evaluation of matrix elements $\langle r^p \rangle$ between nonrelativistic bound-state hydrogenlike wave functions has a long history in quantum mechanics. An incomplete list of references includes [1, 3, 8, 11, 12, 13, 14, 15, 16, 20, 23, 27, 28, 29, 32, 33, 37, 38, 39, 40, 45, 49, 50, 54], and [56] and references therein. Although different methods were used in order to evaluate these matrix elements, one of possible forms of the answer seems has been missing until recently. In Ref. [49] the mean values for states of definite energy

$$\langle r^p \rangle = \frac{\int_{\mathbb{R}^3} |\psi_{nlm}(r)|^2 r^p dv}{\int_{\mathbb{R}^3} |\psi_{nlm}(r)|^2 dv} = \frac{\int_0^\infty R_{nl}^2(r) r^{p+2} dr}{\int_0^\infty R_{nl}^2(r) r^2 dr}, \quad dv = r^2 dr d\omega \quad (2.1)$$

Date: August 6, 2009.

1991 Mathematics Subject Classification. Primary 81Q05, 35C05. Secondary 42A38.

Key words and phrases. The Schrödinger equation, harmonic oscillator, expectation values, Hahn polynomials, hypervirial theorems.
in the nonrelativistic Coulomb problem have been evaluated in terms of the Chebyshev polynomials of a discrete variable $t_k(x, N) = h_k^{(0, 0)}(x, N)$ originally introduced in Refs. [51] and [52]. Their extensions, the so-called Hahn polynomials, introduced also by P. L. Chebyshev [53] and given by

$$h_k^{(\alpha, \beta)}(x, N) = (-1)^k \left( \frac{\Gamma(N)(\beta + 1)}{k!\Gamma(N-k)} \right) \times 3F_2 \left( \begin{array}{ccc} -k, \alpha + \beta + k + 1, -x \\ \beta + 1, 1 - N \end{array} ; 1 \right),$$

were rediscovered and generalized in the late 1940s by W. Hahn. (We use the standard definition of the generalized hypergeometric series throughout the paper [5], [21].)

The end results have the following closed forms

$$\langle r^{k-1} \rangle = \frac{1}{2n} \left( \frac{na_0}{2Z} \right)^{k-1} t_k(n - l - 1, -2l - 1),$$

when $k = 0, 1, 2, ...$ and

$$\langle \frac{1}{r^{k+2}} \rangle = \frac{1}{2n} \left( \frac{2Z}{na_0} \right)^{k+2} t_k(n - l - 1, -2l - 1),$$

when $k = 0, 1, ..., 2l$. Here $a_0 = h^2/me^2$ is the Bohr radius. Equations (2.1)–(2.3) reflect the positivity of the matrix elements under consideration [49].

The ease of handling of these matrix elements for the discrete levels is greatly increased if use is made of the known properties of these classical polynomials of Chebyshev [21], [25], [35], [36] and [51], [52], [53]. The direct consequences of these relations are an inversion relation:

$$\langle \frac{1}{r^{k+2}} \rangle = \left( \frac{2Z}{na_0} \right)^{2k+1} \frac{(2l-k)!}{(2l+k+1)!} \langle r^{k-1} \rangle$$

with $0 \leq k \leq 2l$ and the three-term recurrence relation:

$$\langle r^k \rangle = \frac{2n(2k+1)}{k+1} \left( \frac{na_0}{2Z} \right) \langle r^{k-1} \rangle - k \left( \frac{(2l + 1)^2 - k^2}{k+1} \right) \left( \frac{na_0}{2Z} \right)^2 \langle r^{k-2} \rangle$$

with the initial conditions

$$\langle \frac{1}{r} \rangle = \frac{Z}{\alpha_0 n^2}, \quad \langle 1 \rangle = 1,$$

which is convenient for evaluation of the mean values $\langle r^k \rangle$ for $k \geq 1$.

The recurrence relation (2.6) was originally found by Kramers and Pasternack in the late 1930s [27], [38], and [39]. The inversion relation (2.5), which is also due to Pasternack, has been rediscovered many years later [15], [33] (see also [22] and [23] for historical comments). Generalizations of (2.5)–(2.6) for off-diagonal matrix elements are discussed in Refs. [14], [37], [23], [45], and [50]. The properties of the hydrogenlike radial matrix elements are discussed from a group-theoretical viewpoint in Refs. [3], [16], and [37]. Extensions to the relativistic case are given in [1], [17], [48], and [49] (see also references therein).

In a retrospect, Pasternack’s papers [38], [39] had paved the road to the discovery of the continuous Hahn polynomials in the mid 1980s (see [26], [49] and references therein).
3. Evaluation of $\langle r^p \rangle$ for Harmonic Oscillator in $\mathbb{R}^n$

The stationary Schrödinger equation for the $n$-dimensional harmonic oscillator

$$ H\Psi = E\Psi, \quad H = \frac{1}{2} \sum_{s=1}^{n} \left( -\frac{\partial^2}{\partial x_s^2} + x_s^2 \right) $$

(3.1)

can be solved by separation of the variables in hyperspherical coordinates. The normalized wave functions have the form

$$ \Psi (x) = \Psi_{NK\nu} (r, \Omega) = Y_{K\nu} (\Omega) R_{NK} (r), $$

(3.2)

where $Y_{K\nu} (\Omega)$ are the hyperspherical harmonics associated with a binary tree $T$, the integer number $K$ corresponds to the constant of separation of the variables at the root node of $T$ and $\nu = \{l_1, l_2, \ldots, l_{p_\nu}\}$ is the set of all other subscripts corresponding to the remaining vertexes of the binary tree $T$ (see [35], [46], [47], and [53] for a graphical approach of Vilenkin, Kuznetsov and Smorodinskii to the theory of spherical harmonics).

The radial functions are given by

$$ R_{NK} (r) = \sqrt{\frac{2 ((N-K)/2)!}{\Gamma ((N+K+n)/2)}} \exp \left( -r^2/2 \right) r^K L_{(N-K)/2}^{K+n/2-1} (r^2), $$

(3.3)

where $L_k^\alpha (\xi)$ are the Laguerre polynomials [36] and the corresponding energy levels are equal to

$$ E = E_N = N + n/2, \quad (N-K)/2 = k = 0, 1, 2, \ldots. $$

(3.4)

(See also Refs. [30], [34], [35], [41], and [46] for group theoretical properties of the $n$-dimensional harmonic oscillator wave functions.)

The expectation values under consideration

$$ \langle r^p \rangle = \int_{\mathbb{R}^n} \Psi^*_{NK\nu} (r, \Omega) r^p \Psi_{NK\nu} (r, \Omega) \, dv $$

(3.5)

are derived with the aid of the integral [37, 49]:

$$ J_{nms}^{\alpha\beta} = \int_0^\infty e^{-x} x^{\alpha+s} L_n^\alpha (x) L_m^\beta (x) \, dx $$

(3.6)

$$ = (-1)^{n-m} \frac{\Gamma (\alpha + s + 1) \Gamma (\beta + m + 1) \Gamma (s + 1)}{m! (n-m)! \Gamma (\beta + 1) \Gamma (s - n + m + 1)} $$

$$ \times \; _3F_2 \left( \begin{array}{c} -m, \; s + 1, \; \beta - \alpha - s \\ \beta + 1, \; n - m + 1 \end{array} \right), \; n \geq m, $$

where parameter $s$ may take some integer values. Similar integrals have been discussed in Refs. [1], [17], [18], and [28]. A simple evaluation of this integral is given in Ref. [49].

Indeed,

$$ \langle r^p \rangle = \frac{((N-K)/2)!}{\Gamma ((N+K+n)/2)} \int_0^\infty e^{-\xi \xi^p/2+K+n/2-1} \left( L_{(N-K)/2}^{K+n/2-1} (\xi) \right)^2 d\xi, $$

(3.7)
where we replace \( r^2 = \xi \). As a result,
\[
\langle r^p \rangle = \frac{\Gamma (K + (n + p)/2)}{\Gamma (K + n/2)} \binom{3F2}{(K - N)/2, p/2 + 1, -p/2}{K + n/2, 1, 1}, \tag{3.8}
\]
provided that \( p + n + 2K > 0 \). Connection with the dual Hahn polynomials given by \[35\]
\[
w_m^{(c)} (s(s + 1), a, b) = \frac{(1 + a - b)_m (1 + a + c)_m}{m!} \times \binom{3F2}{-m, a - s, a + s + 1}{1 + a - b, 1 + a + c; 1}.
\tag{3.9}
\]
is as follows
\[
\langle r^p \rangle = \frac{\Gamma (K + (n + p)/2)}{\Gamma ((N + K + n)/2)} \binom{3F2}{(p/2 + 1)}{(p/2 + 1), 0, 1 - K - n/2}.
\tag{3.10}
\]
Thus the direct calculation of \( \langle r^p \rangle \) for each admissible \( p \) involves a well-known special function originally introduced in Ref. \[24\]. Basic properties of the dual Hahn polynomials are discussed in \[35\]. We shall use one of them in the next section. See also Refs. \[16\], \[41\], and \[4\] for group-theoretical methods of evaluation of similar matrix elements. We shall elaborate on the group-theoretical meaning of Eq. (3.8) later.

4. Three Term Recurrence Relation

The difference equation for the dual Hahn polynomials has the form
\[
\sigma (s) \frac{\Delta}{\Delta x} \left( \frac{\nabla y(s)}{\nabla x(s)} \right) + \tau (s) \frac{\Delta y(s)}{\Delta x(s)} + \lambda_m y(s) = 0, \tag{4.1}
\]
where \( \Delta f(s) = \nabla f(s + 1) - f(s), \ x(s) = s(s + 1), \ x_1(s) = x(s + 1/2), \) and
\[
\sigma (s) = (s - a) (s + b) (s - c),
\tag{4.2}
\]
\[
\sigma (s) + \tau (s) \nabla x_1(s) = \sigma (-s - 1)
\tag{4.3}
\]
\[
= (a + s + 1) (b - s - 1) (c + s + 1),
\]
\[
\lambda_m = m. \tag{4.4}
\]
It can be rewritten as a recurrence relation
\[
\sigma (-s - 1) \nabla x(s) y(s + 1) + \sigma (s) \Delta x(s) y(s - 1) \tag{4.5}
\]
\[
+ (\lambda_m \Delta x(s) \nabla x(s) \nabla x_1(s) - \sigma (-s - 1) \nabla x(s) - \sigma (s) \Delta x(s)) y(s) = 0.
\]
See \[24\], \[25\] and \[35\] for more details on the properties of the dual Hahn polynomials.

Equations (3.10) and (4.5) results in the three-term recurrence relation
\[
(p + 2) \langle r^{p+2} \rangle = (p + 1) (2N + n) \langle r^p \rangle \tag{4.6}
\]
\[
+ p \left( \frac{p^2 - n^2}{4} - (K - 1)(K + p - 1) \right) \langle r^{p-2} \rangle
\]
for the matrix elements. Such recurrence relation requires two initial results
\[
\langle 1 \rangle = 1, \quad \langle \frac{1}{r^2} \rangle = \frac{1}{K + n/2 - 1}. \tag{4.7}
\]
in order to generate all expectation values.

The cases \( n = 1, 2, 3 \) are well-known and usually discussed with the help of the hypervirial theo-

rems (see, for example, \([4], [11], [20], [7], [40]\), and references therein.) Our approach emphasizes the

simple fact that the matrix elements recurrence relations (2.6) and (4.6) for the hydrogen atom and

for the \( n \)-dimensional harmonic oscillator, respectively, have the same “special functions” nature,

namely, they occur due to the difference equation for the corresponding dual Hahn polynomials.

We leave further details to the reader.

5. A Pasternack-Type Inversion Property

From equation (3.8) one gets

\[
\langle r^{-p-2} \rangle = \frac{\Gamma(K + (n-p)/2 - 1)}{\Gamma(K + (n+p)/2)} \langle r^p \rangle \tag{5.1}
\]

(for all the convergent integrals) in the spirit of Pasternack’s inversion relation (2.5) valid in the case

of the hydrogen atom. It simply reflects an obvious fact that the argument \( x(p) = (p/2 + 1)p/2 \)

of the dual Hahn polynomials in (3.10) obeys a natural symmetry \( x(-p-2) = x(p) \) on the corre-

sponding quadratic grid. We were unable to find relations (3.8), (3.10), and (5.1) in the available

literature.

6. A Conclusion

Special functions appear in numerous applications of mathematical and physical sciences and

their basic knowledge is a necessity for any theoretical physicist. As Dick Askey mentioned once in

his talk on mathematical education, “We should not lie to our students, but we do not have to tell

them the whole truth.” The same is true about teaching elementary topics in quantum mechanics.

As we can conclude from this short note, even if “one is able to evaluate average values by appeal to
general principles rather that by direct integration [20]”, important relations with the well-known

special functions will be out of the picture due to the limiting mathematical tools. Every instructor

has to find a way how to resolve this contradiction.

Acknowledgment. This paper is written as a part of the summer 2009 program on analysis of
Mathematical and Theoretical Biology Institute (MTBI) and Mathematical, Computational and
Modeling Sciences Center (MCMSC) at Arizona State University. The MTBI/SUMS Summer Under-
graduate Research Program is supported by The National Science Foundation (DMS-0502349),
The National Security Agency (dod-h982300710096), The Sloan Foundation, and Arizona State
University. We thank Professor Carlos Castillo-Chávez for support, valuable discussions and en-
couragement. One of the authors (RCS) is supported by the following National Science Foundation
programs: Louis Stokes Alliances for Minority Participation (LSAMP): NSF Cooperative Agree-
ment No. HRD-0602425 (WAESO LSAMP Phase IV); Alliances for Graduate Education and the
Professoriate (AGEP): NSF Cooperative Agreement No. HRD-0450137 (MGE@MSA AGEP Phase II).
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\[ \langle r^p \rangle \text{ for Harmonic Oscillator in } \mathbb{R}^n \]

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