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Quantum expectation values of *D*-dimensional Rydberg hydrogenic states by use of Laguerre and Gegenbauer asymptotics

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Abstract
The radial position ($\langle r^{\alpha}\rangle$, $\alpha \in \mathbb{R}$) and momentum ($\langle p^{\beta}\rangle$, $\beta \in (-1,\ 3)$) expectation values of the *D*-dimensional Rydberg hydrogenic states (i.e. states where the electron has a large hyperquantum number *n*) are rigorously determined by means of powerful tools of the modern approximation theory relative to the asymptotics of the varying orthogonal Laguerre and Gegenbauer polynomials which control the corresponding wavefunctions in position and momentum spaces.

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1. Introduction

The *D*-dimensional hydrogenic system with nuclear charge *Z* [1–4] is not only the main prototype of *D*-dimensional physics [5, 6] but it also plays a relevant role in numerous phenomena of quantum field theory [7], quantum chemistry [1, 5, 6, 8], quantum computation [9] and nanotechnology [10, 11]. Beyond the three-dimensional hydrogen atom, the existence of hydrogenic systems with dimensionality other than 3 has been observed for $D < 3$ [10] and suggested for $D > 3$ [12]. Usually this problem is treated, as we will do here, by using the standard Coulomb potential for the electron–proton interaction in all dimensions because it is both valuable and appropriate for understanding numerous physical phenomena. Nevertheless, we should point out that other authors have indicated that Gauss' law gives a different potential (one that describes the flux due to a point source) which explicitly depends upon the dimension (see e.g. [13]); in two-dimensional space this potential is a logarithmic function of the distance separating the two particles [14].

The physical solutions of the corresponding Schrödinger equation, which describe the wavefunctions of the quantum mechanically allowed states of the system, have been exactly determined in both position [1, 3, 4] and momentum [15] spaces mainly because the associated potential energy has the Coulomb form $V(\vec{r}) = -Z/r$, $r = |\vec{r}|$. The analytic expressions for the wavefunctions are controlled by the Laguerre and Gegenbauer orthogonal polynomials in position space, and only by the Gegenbauer polynomials in momentum space, as it is briefly reminded in section 2.

The expectation values of arbitrary powers of the position and momentum coordinates (hereafter to be denoted by $\langle r^\alpha \rangle$ and $\langle p^\alpha \rangle$, respectively) are the basic elements of the D-dimensional hydrogenic system. This is so not only because they characterize the quantum probability densities of the system in the two reciprocal spaces, but also because they determine various fundamental quantities (diamagnetic susceptibility, kinetic energy, etc) and/or tightly bound the macroscopic properties of the system [16].

This work focuses on the position and momentum expectation values of highly excited (Rydberg) D-dimensional hydrogenic states. These states play a relevant role in the D-dimensional physics [5] and Rydberg physics of atoms and molecules [17–19]. We calculate the expectation values $\langle r^\alpha \rangle$ and $\langle p^\alpha \rangle$ of these Rydberg states by means of a methodology based on powerful tools of the modern approximation theory relative to the asymptotics $(n \to \infty)$ of the Laguerre $\tilde{L}_n^\alpha(x)$ and Gegenbauer $\tilde{C}_n^\alpha(x)$ orthogonal polynomials [20]. Let us advance saying that our results considerably improve the values obtained by the semiclassical approximation and other means [21] for these quantities.

The paper is organized as follows. In section 2, we gather the basic properties of the D-dimensional hydrogenic problem which are needed for the rest of the work. In section 3, we calculate the position expectation values $\langle r^\alpha \rangle$ of the Rydberg states by use of the asymptotics of varying Laguerre polynomials. In section 4, we find the momentum expectation values $\langle p^\alpha \rangle$ of the Rydberg states by use of the asymptotics of varying Gegenbauer polynomials. Finally some open problems and conclusions are given.

2. The *D*-dimensional hydrogenic problem: generalities

In this section, we briefly describe the bound states of the hydrogenic system in D dimensions. We give their wavefunctions, probability densities and radial expectation values in the position and momentum spaces. These states are characterized by the D integer hyperquantum numbers

$$(n, \mu_1 \equiv l, \mu_2, \ldots, \mu_{D-1}) \equiv (n, l, \{\mu\}),$$

where n denotes the principal hyperquantum number and $(l, \{\mu\})$ are the $D-1$ hyperquantum numbers associated with the angular variables $\Omega_{D-1} \equiv (\theta_1, \theta_2, \ldots, \theta_{D-1})$ which may have all values consistent with the inequalities $l \equiv \mu_1 \geqslant \mu_2 \geqslant \cdots \geqslant |\mu_{D-1}| \equiv |m| \geqslant 0$. Atomic units will be used throughout the paper.

The wavefunction of the bound states $(n, l, \{\mu\})$ in position space has the form [2–4] $\Psi(\vec{r}, t) = \psi(\vec{r}) \exp(-\mathrm{i} E_\eta t)$, with

$$E_\eta = -\frac{Z^2}{2\eta^2}, \qquad \eta = n + \frac{D-3}{2}, \qquad n = 1, 2, 3, \ldots, \tag{1}$$

for the energy, and

$$\Psi_{n,l,\{\mu\}}(\vec{r}) = R_{n,l}(r)\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1}) \tag{2}$$

for the eigenfunctions expressed in spherical coordinates $\vec{r} = (r, \theta_1, \theta_2, \dots, \theta_{D-1} \equiv \phi) = (r, \Omega_{D-1})$ where $r = \left(x_1^2 + \dots + x_D^2\right)^{1/2}$, x_i being the ith Cartesian coordinate. The radial part is

$$R_{n,l}(r) = \left[\frac{1}{2\eta}\left(\frac{2Z}{\eta}\right)^D\right]^{1/2} t^{-\frac{D-2}{2}}\sqrt{\omega_{2L+1}(t)}\tilde{\mathcal{L}}^{(2L+1)}_{\eta-L-1}(t), \tag{3}$$

where $\omega_\alpha(t) = t^\alpha\, \mathrm{e}^{-t}$, $t = \frac{2Zr}{\eta}$, $L = l + \frac{D-3}{2}$ and $\tilde{\mathcal{L}}^\alpha_k(x)$ denotes the Laguerre polynomial of degree k and parameter α, orthonormal on $[0, +\infty)$ with respect to ω_α. It is worth noting that $2L + 1 = 2l + D - 2$ and $\eta - L - 1 = n - l - 1$, so that $\tilde{\mathcal{L}}^{2L+1}_{\eta-L-1}(t) = \tilde{\mathcal{L}}^{2l+D-2}_{n-l-1}(t)$.

The angular part is given by the hyperspherical harmonics [6]

$$\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1}) = \frac{1}{\sqrt{2\pi}}\,\mathrm{e}^{\mathrm{i}m\varphi}\prod_{j=1}^{D-2}\tilde{C}^{(\alpha_j+\mu_{j+1})}_{\mu_j-\mu_{j+1}}(\cos\theta_j)(\sin\theta_j)^{\mu_{j+1}}, \tag{4}$$

where $\alpha_j = (D - j - 1)/2$, and $\tilde{C}^\alpha_k(x)$ denotes the Gegenbauer polynomial of degree k and parameter α, orthonormal on the interval $[-1, +1]$ with respect to the weight $\omega^*_\alpha(x) = (1 - x^2)^{\alpha-\frac{1}{2}}$. Then, the corresponding quantum–mechanical probability density $\rho(\vec{r}) = |\Psi(\vec{r}, t)|^2 = |\psi_{n,l,\{\mu\}}(\vec{r})|^2$ is given by

$$\begin{aligned}\rho(\vec{r}) &= R^2_{n,l}(r)|\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})|^2\\ &= \frac{1}{2\eta}\left(\frac{2Z}{\eta}\right)^D t^{-(D-2)}\omega_{2L+1}(t)\left[\tilde{\mathcal{L}}^{(2L+1)}_{\eta-L-1}(t)\right]^2|\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})|^2.\end{aligned} \tag{5}$$

This density function is characterized by the knowledge of its radial expectation values $\langle r^\alpha\rangle$ defined by

$$\begin{aligned}\langle r^\alpha\rangle &= \int r^\alpha\rho(\vec{r})\,\mathrm{d}^D r = \int_0^\infty r^{\alpha+D-1}R^2_{n,l}(r)\,\mathrm{d}r\\ &= \frac{1}{2\eta}\left(\frac{\eta}{2Z}\right)^\alpha\int_0^\infty\omega_{2L+1}(t)\left[\tilde{\mathcal{L}}^{(2L+1)}_{\eta-L-1}(t)\right]^2 t^{\alpha+1}\,\mathrm{d}t\end{aligned} \tag{6}$$

where we have taken into account equation (5) and the orthogonality relation of the hyperspherical harmonics [6] for the second equality, and equation (3) in the third equality. It is worth pointing out that this functional of the Laguerre polynomials can be expressed [4, 22, 23] in terms of (η, L) by means of a generalized hypergeometric function with unit argument of the form ${}_3F_2(1)$, allowing for the explicit evaluation for the expectation values with the lowest powers. Moreover, some recursion relations are also known [4, 22–24].

In the momentum space, the wavefunctions [4, 15] of the state $(n, l, \{\mu\})$ are given by $\Phi(\vec{p}, t) = \phi(\vec{p})\exp(-\mathrm{i}E_\eta t)$, where $\phi(\vec{p})$ is the Fourier transform of the position eigenfunction $\psi(\vec{r})$, which has the expression

$$\tilde{\phi}_{n,l\{\mu\}}(\vec{p}) = \mathcal{M}_{n,l}(p)\mathcal{Y}_{l\{\mu\}}(\Omega'_{D-1}), \tag{7}$$

where $\vec{p} = (p, \theta'_1, \theta'_2, \dots, \theta'_{D-1}) \equiv (p, \Omega'_{D-1})$ with $p = \left(p_1^2 + \dots + p_D^2\right)^{1/2}$, p_i being the ith momentum Cartesian coordinate. The radial part turns out to be (with the notation introduced above)

$$\mathcal{M}_{n,l}(p) = \left(\frac{\eta}{Z}\right)^{D/2}(1 + y)^{3/2}\left(\frac{1 + y}{1 - y}\right)^{\frac{D-2}{4}}\sqrt{\omega^*_{L+1}(y)}\tilde{C}^{(L+1)}_{\eta-L-1}(y) \tag{8}$$

with $y = (1-\eta^2\tilde{p}^2)/(1+\eta^2\tilde{p}^2)$, $\tilde{p} = p/Z$ and, as before, $\omega^*_\alpha(y) = (1-y^2)^{\alpha-\frac{1}{2}}$. The angular part is again an hyperspherical harmonics of the type (4). Then, the momentum probability density of the D-dimensional hydrogenic system $\gamma(\vec{p}) = |\Phi(\vec{p},t)|^2 = |\phi(\vec{p})|^2$ is given by

$$\gamma(\vec{p}) = \mathcal{M}^2_{n,l}(p)|\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})|^2. \tag{9}$$

The radial expectation values $\langle p^\alpha\rangle$ of this momentum density are

$$\begin{aligned}\langle p^\alpha\rangle &:= \int p^\alpha \gamma(\vec{p})\,\mathrm{d}^D p = \int_0^\infty p^{\alpha+D-1}\mathcal{M}^2_{n,l}(p)\,\mathrm{d}p \\ &= \left(\frac{Z}{\eta}\right)^\alpha \int_{-1}^{1} \omega^*_{L+1}(t)\big[\tilde{C}^{(L+1)}_{\eta-L-1}(t)\big]^2 (1-t)^{\frac{\alpha}{2}}(1+t)^{1-\frac{\alpha}{2}}\,\mathrm{d}t\end{aligned} \tag{10}$$

for all values of α within the range $-2l-D \leqslant \alpha \leqslant 2l+D+2$. Again, this functional of Gegenbauer polynomials can be expressed [25] as a function of (α,η,L) in terms of a generalized hypergeometric function ${}_5F_4$ with unit argument, allowing us to find some recursion relations for $\langle p^\alpha\rangle$ as well as the explicit values for $\alpha = 0, 2$ and 4 [4, 25]. See also [26] for the three-dimensional case.

3. Position expectation values $\langle r^\alpha\rangle$ for Rydberg states

In this section, we calculate the radial expectation values in the position space, $\langle r^\alpha\rangle$, $\alpha\in\mathbb{R}$, for highly excited or Rydberg states (i.e. for states with large principal hyperquantum number n) of D-dimensional hydrogenic systems. For an arbitrary $(n,l,\{\mu\})$-state, we know from equation (6) that

$$2\eta\left(\frac{2Z}{\eta}\right)^\alpha\langle r^\alpha\rangle = \int_0^\infty \omega_{\nu'}(t)\big[\tilde{\mathcal{L}}^{(\nu')}_k(t)\big]^2 t^{\alpha+1}\,\mathrm{d}t \tag{11}$$

with $k = \eta-L-1 = n-l-1$ and $\nu' = 2L+1 = 2l+D-2$. Note that this integral converges for all values of $\alpha > -2l-D$. With the change $t\to x : t = kx$, one has that

$$2\eta\left(\frac{2Z}{\eta}\right)^\alpha\langle r^\alpha\rangle = k^{\alpha+1}\int_0^\infty x^{\nu'}\mathrm{e}^{-kx}\big[\hat{\mathcal{L}}^{(\nu')}_{k,k}(x)\big]^2 x^{\alpha+1}\,\mathrm{d}x, \tag{12}$$

where the polynomial

$$\hat{\mathcal{L}}^{(\nu')}_{k,k}(x) \equiv k^{\frac{\nu'+1}{2}}\tilde{\mathcal{L}}^{(\nu')}_k(kx) \tag{13}$$

is orthonormal on $[0,+\infty)$ with respect to the weight $x^{\nu'}\mathrm{e}^{-kx}$. We need to analyze its asymptotics as $n\to\infty$. For that, we assume that $l\in\{0,1,\ldots,n-1\}$ varies in such a way that the limit

$$\lim_{n\to\infty}\frac{l}{n} = s\in[0,1) \tag{14}$$

exists (clearly, the case of l constant is included). In particular, $k\to\infty$ if and only if $n\to\infty$, and

$$\lim_{k\to\infty}\frac{\nu'}{k} = \frac{2s}{1-s}\in[0,+\infty).$$

With these assumptions the polynomials in (13) are orthogonal with respect to a varying weight, i.e. a weight which depends on the degree k in the form

$$\omega_k(x) = x^{\alpha_k}\mathrm{e}^{-\beta_k x} \qquad \text{with} \qquad \alpha_k = \nu' \quad\text{and}\quad \beta_k = k. \tag{15}$$

According to Buyarov *et al* [20, corollary 5], in the weak-* sense[6]

$$\left[\hat{\mathcal{L}}_{k,k}^{(\nu')}(x)\right]^2\omega_k(x) \longrightarrow \mathrm{d}\mu_{[a,b]}(x) := \frac{\mathrm{d}x}{\pi\sqrt{(x-a)(b-x)}}, \qquad \text{for} \quad k\to\infty, \tag{16}$$

where

$$a=\frac{2}{1-s}\left(1-\sqrt{1-s^2}\right), \qquad b=\frac{2}{1-s}\left(1+\sqrt{1-s^2}\right). \tag{17}$$

Hence,

$$\lim_{k\to\infty}\int_0^\infty x^{\nu'}\mathrm{e}^{-kx}\left[\hat{\mathcal{L}}_{k,k}^{(\nu')}(x)\right]^2x^{\alpha+1}\mathrm{d}x = \frac{1}{\pi}\int_a^b\frac{x^{\alpha+1}}{\sqrt{(x-a)(b-x)}}\,\mathrm{d}x. \tag{18}$$

With the change of variable $z=(x-a)/(b-a)$, the last integral can be transformed into

$$\begin{aligned}\lim_{k\to\infty}\int_0^\infty & x^{\nu'}\mathrm{e}^{-kx}\left[\hat{\mathcal{L}}_{k,k}^{(\nu')}(x)\right]^2x^{\alpha+1}\,\mathrm{d}x\\ &=\frac{a^{\alpha+1}}{\pi}\int_0^1 z^{-\frac{1}{2}}\,(1-z)^{-\frac{1}{2}}\left(1+\frac{b-a}{a}z\right)^{\alpha+1}\,\mathrm{d}z\\ &=a^{\alpha+1}{}_2F_1\left(-1-\alpha,\frac{1}{2},1,\frac{a-b}{a}\right),\end{aligned} \tag{19}$$

where we have used the following integral representation of the hypergeometric function ${}_2F_1(z)$:

$${}_2F_1\,(a,b,c,z)=\frac{\Gamma(c)}{\Gamma(c-b)\Gamma(b)}\int_0^1 t^{b-1}(1-t)^{c-b-1}(1-zt)^{-b}\,\mathrm{d}t.$$

Using equation (12) we obtain

$$\lim_{k\to\infty}2\eta\left(\frac{2Z}{\eta}\right)^\alpha\langle r^\alpha\rangle=(ak)^{\alpha+1}{}_2F_1\left(-1-\alpha,\frac{1}{2},1,\frac{a-b}{a}\right). \tag{20}$$

Taking into account that $\eta=n+\frac{D-3}{2}$ and $k=\eta-L-1=n-l-1$ and equation (17), we find

$$\begin{aligned}\left(\frac{Z}{\eta^2}\right)^\alpha\langle r^\alpha\rangle &\simeq \left(1-\sqrt{1-s^2}\right)^{\alpha+1}\\ &\times{}_2F_1\left(-1-\alpha,\frac{1}{2},1,\frac{2\left(-1+s^2-\sqrt{1-s^2}\right)}{s^2}\right), \qquad n\to\infty.\end{aligned} \tag{21}$$

Let us analyze in more detail the case when l is uniformly bounded, which implies that $s=0$, $a=0$, $b=4$, and we get

$$\lim_{k\to\infty}\int_0^\infty x^{\nu'}\mathrm{e}^{-kx}\left[\hat{\mathcal{L}}_{k,k}^{(\nu')}(x)\right]^2x^{\alpha+1}\,\mathrm{d}x=\frac{1}{\pi}\int_0^4\frac{x^{\alpha+1/2}}{\sqrt{4-x}}\,\mathrm{d}x=\frac{\Gamma\left(\alpha+\frac{3}{2}\right)}{\sqrt{\pi}\,\Gamma(\alpha+2)}, \tag{22}$$

so that using it in equation (12), we finally obtain

$$\lim_{k\to\infty}2\eta\left(\frac{2Z}{\eta}\right)^\alpha\langle r^\alpha\rangle=\frac{(4k)^{\alpha+1}}{\sqrt{\pi}}\frac{\Gamma\left(\alpha+\frac{3}{2}\right)}{\Gamma(\alpha+2)}, \tag{23}$$

which describes the radial expectation values $\langle r^\alpha\rangle$ of Rydberg hydrogenic states, namely states with uniformly bounded (α, l, D) and $n\to\infty$.

[6] We should point out that the result in [20] is stated under an assumption that $\lim_k \alpha_k/k>0$. However, it is easily seen that it is also valid when this limit is 0.

Taking into account that $\eta = n + \frac{D-3}{2}$ and $k = \eta - L - 1 = n - l - 1$, equation (23) can be rewritten as

$$\left(\frac{Z}{\eta^2}\right)^{\alpha} \langle r^{\alpha}\rangle \simeq \frac{2^{\alpha+1}\Gamma\left(\alpha+\frac{3}{2}\right)}{\sqrt{\pi}\,\Gamma(\alpha+2)}, \qquad n \to \infty; \tag{24}$$

observe that the right-hand side is finite for $\alpha > -3/2$. This expression corroborates the corresponding semiclassical and quantum values obtained previously [21] in the three-dimensional case by completely different means.

From equation (24), we obtain

$$\langle r^{-1}\rangle = \frac{Z}{\eta^2}, \qquad \langle r^{0}\rangle = 1, \qquad \langle r\rangle \simeq \frac{3\eta^2}{2Z}, \qquad \langle r^{2}\rangle \simeq \frac{5}{2}\left(\frac{\eta^2}{Z}\right)^2$$

for the first few expectation values of the Rydberg hydrogenic system in agreement with the results of Ray *et al* [24] and Tarasov [22]; in fact, the first two expressions are exact.

If $s > 0$ in equation (14), then the asymptotic expression in equation (19) makes sense for any $\alpha \in \mathbb{R}$. As we observed before, this is not the case when $s = 0$ (i.e. for finite l and $n \to \infty$): the asymptotics in equation (24) is valid for $\alpha > -3/2$, while the right-hand side in equation (11) makes sense for $\alpha > -2l - D$. This gap can be traced back to the weak-$*$ asymptotic formula (16). To extend the result (24) when $s = 0$ to the missing values of α, we can either use finer asymptotic results for the Laguerre polynomials (such as their strong asymptotics, in the spirit of [27, 28]) or follow a different approach that we illustrate next.

The problem of the determination of the asymptotics of the expectation value of the negative powers of r from the critical value $-\frac{3}{2}$ down to $-2l - D$ is very relevant in the three-dimensional case for the analysis of the energy and other atomic properties of Rydberg atoms consisting of an electron in a high-(nl) quantum state moving in the field of a polarizable core; in particular, they control the ionization energy of the Rydberg electron, as first shown by Drachman [29]. This problem can be solved for any dimensionality by taking into account the following connection formula between the expectation values of the positive and negative powers of r found by various authors (see e.g. [24, 29]):

$$\langle r^{-q}\rangle = \left(\frac{2Z}{\eta}\right)^{2q-3} \frac{\Gamma(2L+3-q)}{\Gamma(2L+q)} \langle r^{q-3}\rangle. \tag{25}$$

This expression together with equation (24) allows us to find the asymptotics

$$\langle r^{-q}\rangle \simeq \frac{Z^q}{\eta^3}\frac{\Gamma(2L-q+3)}{\Gamma(2L+q)}\frac{2^{3q-5}\Gamma\left(q-\frac{3}{2}\right)}{\sqrt{\pi}\,\Gamma(q-1)}, \qquad n \to \infty, \tag{26}$$

valid for $q \in (3/2, 2L+3)$. In this way, we cover the full range of the admissible parameters α, except for the critical value $\alpha = -3/2$. In particular, equation (26) with $q = 2$ and 3 provides the exact values

$$\langle r^{-2}\rangle = \frac{Z^2}{\eta^3\left(L+\frac{1}{2}\right)}, \qquad \langle r^{-3}\rangle = \frac{Z^3}{\eta^3(L+1)\left(L+\frac{1}{2}\right)L},$$

as well as for $q = 4$ yields

$$\langle r^{-4}\rangle \simeq \frac{3Z^4}{2\eta^3\left(L+\frac{3}{2}\right)(L+1)\left(L+\frac{1}{2}\right)L\left(L-\frac{1}{2}\right)}$$

for all Rydberg states ($n \to \infty$).

4. Momentum expectation values $\langle p^\alpha \rangle$ for Rydberg states

We can turn now to the radial expectation values in the momentum space, $\langle p^\alpha \rangle$, $\alpha \in \mathbb{R}$, for the Rydberg states (i.e. states with large n). We begin with equation (10) for the expectation values $\langle p^\alpha \rangle$ of an arbitrary state with quantum numbers $(n, l, \{\mu\})$, which may be rewritten as

$$\left(\frac{\eta}{Z}\right)^\alpha \langle p^\alpha \rangle = \int_{-1}^{1} \omega_\nu^*(t)\left[\tilde{C}_k^{(\nu)}(t)\right]^2 (1-t)^{\frac{\alpha}{2}} (1+t)^{1-\frac{\alpha}{2}}\, \mathrm{d}t \tag{27}$$

where $k = \eta - L - 1 = n - l - 1$, $\nu = L + 1 = l + \frac{D-1}{2}$ and $\omega_\nu^*(t) = (1-t^2)^{\nu-\frac{1}{2}}$. Observe that this integral converges only when $-2\nu - 1 < \alpha < 2\nu + 3$, i.e. when $-2l - D < \alpha < 2l + D + 2$.

Again, we need to study the asymptotics of the integrand in (27) when $n \to \infty$ in such a way that (14) holds. In this case, the Gegenbauer polynomials $\tilde{C}_k^\nu(t)$ are orthonormal with respect to a weight which eventually depends on k (varying weight). However, under assumptions (14), the weak-$*$ asymptotics of these polynomials is known, see [20, 30]. Indeed, by equation (14) and [20, corollary 4],

$$\omega_\nu^*(t)\left[\tilde{C}_k^{(\nu)}(t)\right]^2 \longrightarrow \mathrm{d}\mu_{[a,b]}(x), \qquad \text{for} \quad k \to \infty, \tag{28}$$

in the weak-$*$ sense, but now

$$b = -a = \frac{\sqrt{1+2s}}{1+s} \in \left(\frac{\sqrt{3}}{2}, 1\right].$$

Hence, equation (27) implies that

$$\lim_{k\to\infty}\left(\frac{\eta}{Z}\right)^\alpha \langle p^\alpha \rangle = \frac{1}{\pi}\int_{-b}^{b} \frac{(1-t)^{\frac{\alpha}{2}}(1+t)^{1-\frac{\alpha}{2}}}{\sqrt{b^2 - t^2}}\, \mathrm{d}t, \tag{29}$$

and the right-hand side makes sense for any real α as long as $s > 0$.

If l is uniformly bounded, we obtain $s = 0$ and $b = 1$, so that

$$\lim_{k\to\infty}\left(\frac{\eta}{Z}\right)^\alpha \langle p^\alpha \rangle = \frac{1}{\pi}\int_{-1}^{+1} \left(\frac{1-t}{1+t}\right)^{\frac{\alpha-1}{2}} \mathrm{d}t$$
$$= \begin{cases} \dfrac{\alpha - 1}{\sin(\pi(\alpha-1)/2)}, & -1 < \alpha < 3, \quad \alpha \neq 1, \\ 2/\pi, & \alpha = 1, \end{cases} \tag{30}$$

where $\eta = n + \frac{D-3}{2}$. This gives us the asymptotics for the momentum expectation values of the Rydberg states $(n, l, \{\mu\})$ of a D-dimensional hydrogenic system with uniformly bounded $(l, \{\mu\}, D)$. Note that for the integer values $\alpha = 0$, 1 and 2, this expression renders the exact values

$$\langle p^0 \rangle = 1, \qquad \langle p \rangle = \frac{2Z}{\pi\eta}, \qquad \langle p^2 \rangle = \frac{Z^2}{\eta^2}$$

for the normalization of the momentum wavefunction (7), the centroid of the momentum density and for the kinetic energy of the system, respectively.

However, as it happened for the position expectation values, the expression in equation (30) is valid only for a subrange $\alpha \in (-1, 3)$ of all possible values of the parameter α, i.e. $-2l - D < \alpha < 2l + D + 2$. Again, this gap can be traced back to the weak-$*$ asymptotic formula (28). Hence, to extend the result (30) to the missing values of α, we could think of using a recurrence of the form (25). Unfortunately, the only available connection formula between positive and negative powers is

$$\langle p^{-\beta} \rangle = \left(\frac{\eta}{Z}\right)^{2\beta+2} \langle p^{\beta+2} \rangle, \qquad \beta = 0, 1, 2, \ldots$$

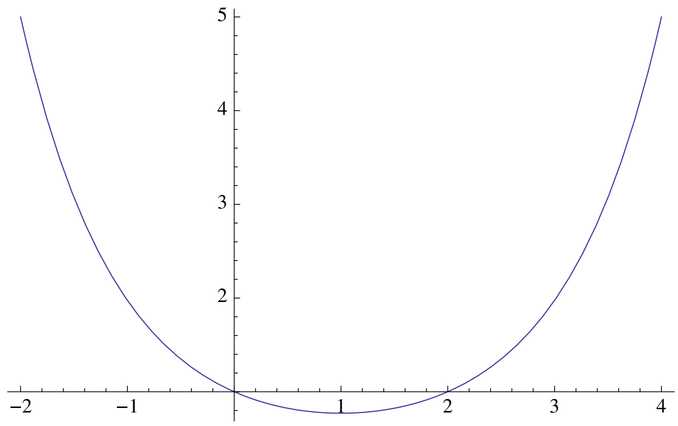

Figure 1. Plot of the function on the right-hand side of (31) for $\alpha \in (-2, 4)$.

Observe that the mapping $-\beta \mapsto \beta + 2$ preserves the interval $(-1, 3)$, so this approach does not take us too far. The problem of finding an asymptotic expression for the moments outside of the range $\alpha \in (-1, 3)$ remains open except for the case $\alpha = -1$ which has been recently analyzed [31] in a detailed way.

Finally, motivated by the modern achievements of Rydberg physics [19], we mention the problem of the asymptotics of $\langle p^\alpha \rangle$ for D-dimensional states $(n, l, \{\mu\})$ when $(D, \{\mu\})$ are bounded, and both n and l tend to infinity in such a way that $n - l$ =constant. Observe that this case corresponds to the value $s = 1$ in equation (14). From equation (29) we could heuristically infer that

$$\lim_{n\to\infty} \left(\frac{\eta}{Z}\right)^\alpha \langle p^\alpha \rangle = \frac{1}{2\pi} \int_{-1}^{1} \frac{(2 - \sqrt{3}t)^{\frac{\alpha}{2}} (2 + \sqrt{3}t)^{1-\frac{\alpha}{2}}}{\sqrt{1 - t^2}} \, \mathrm{d}t, \tag{31}$$

which gives us the first term of the asymptotics. The plot of the right-hand side as a function of α is given in figure 1.

Let us also point out that for the particular cases $\alpha = 0$ and $\alpha = 2$, we obtain the exact values of $\langle p^0 \rangle$ and $\langle p^2 \rangle$, previously given. In summary, the cases (i) $s > 0$ and (ii) $s = 1$ assuming $l \to \infty$, are fully solved by means of equations (29) and (31), respectively; the case $s = 0$ (i.e. when l is finite and $n \to \infty$) is open.

5. Conclusions

The position and momentum expectation values of $\langle r^\alpha \rangle$ and $\langle p^\beta \rangle$ of D-dimensional Rydberg hydrogenic states ($n \to \infty$) are rigorously determined in terms of D and the hyperquantum principal and orbital quantum numbers; when $l = o(n)$, the values of α and β should be restricted to $\alpha \neq -3/2$ and $\beta \in (-1, 3)$. We have used the asymptotics of the Laguerre and Gegenbauer polynomials, which control the position and momentum wavefunctions, respectively, of the Rydberg state. It is worth noting that their parameters (hence, their orthogonality weights) depend on the polynomial degree, so that standard asymptotic results are not applicable.

The calculation of $\langle p^\beta \rangle$ with $\beta \notin (-1, 3)$ remains open and probably requires the use of finer asymptotic results for the orthogonal polynomials, such as e.g. their strong asymptotics in the spirit of Aptekarev *et al* [27]. It is interesting to mention here that the case $\beta = -1$ has been solved [31] in 2009, though not completely since the regime when $s = l/n$ is finite still remains open.

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