

INFORMATION ENTROPY OF CLASSICAL ORTHOGONAL POLYNOMIALS AND THEIR APPLICATION TO THE HARMONIC OSCILLATOR AND COULOMB POTENTIALS

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ABSTRACT. The information entropy is explicitly obtained for the harmonic oscillator and the hydrogen atom (Coulomb potential) in D dimensions ($D = 1, 2, 3$). It is shown how these entropies are related to entropies involving classical orthogonal polynomials and the physical interpretation of this information entropy is given.

1. Introduction

The Schrödinger equation in D dimensions with radially symmetric potential V is given in atomic units by

$$\left(-\frac{1}{2}\nabla^2 + V(r)\right)\psi = E\psi$$

where

$$r^2 = \sum_{j=1}^D x_j^2.$$

For the harmonic oscillator, the potential is

$$V(r) = \frac{1}{2}\lambda^2 r^2,$$

and for the hydrogen atom, we use the Coulomb potential

$$V(r) = -\frac{1}{r}.$$

The information entropy for these physical systems is given by

$$S_\rho = - \int \rho(\vec{r}) \log \rho(\vec{r}) d\vec{r} \tag{1.1}$$

in the position space where $\rho(\vec{r}) = |\psi(\vec{r})|^2$ is the density corresponding to the wave function $\psi(\vec{r})$ and

$$S_\gamma = - \int \gamma(\vec{p}) \log \gamma(\vec{p}) d\vec{p} \tag{1.2}$$

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in the momentum space where $\gamma(\vec{p}) = |\hat{\psi}(\vec{p})|^2$ is the density corresponding to the wave function $\hat{\psi}(\vec{p})$, which is the Fourier transform of $\psi(\vec{r})$.

These two entropies have allowed Bialynicki-Birula and Mycielski [6] to find a new and stronger version of the Heisenberg uncertainty relation. For a quantum mechanical system in D dimensions, this uncertainty relation is

$$S_\rho + S_\gamma \geq D(1 + \log \pi), \quad (1.3)$$

which expresses in a quantitative way the property that it is impossible to get precise information of such a system in both position and momentum space: high values of S_ρ are associated with low values of S_γ , and vice versa. To get some idea of the restriction this gives to the systems under consideration, one would require good estimates and bounds for the entropies, such as those given in [1]. For the fundamental quantum mechanical systems considered in this paper, i.e., the harmonic oscillator and the hydrogen atom, the entropies are in terms of classical orthogonal polynomials. They can be expressed by means of integrals of the form

$$\int p_n^2(x) \log p_n^2(x) d\mu(x) \quad (1.4)$$

where $p_n(x)$ are orthogonal polynomials with respect to a measure μ . The orthogonal polynomials that appear are the Gegenbauer polynomials, the Laguerre polynomials, and the Hermite polynomials. Since quite a lot is known for these special functions, one hopes to be able to find a relatively simple closed expression for integrals of the form (1.4). We show how the entropy (1.4) is related to the logarithmic potential of the measure $p_n^2(x) d\mu(x)$ and give a simple recursive relation for these logarithmic potentials for Gegenbauer polynomials, Laguerre polynomials, and Hermite polynomials. These results extend the work in [19] and [3]. The analysis of entropy integrals (1.4) for weights on $(-\infty, \infty)$ is given in [18], and the asymptotic behaviour for general orthogonal polynomials is given in [2, 4].

2. The D -dimensional harmonic oscillator

For the harmonic oscillator in D dimensions, the potential is

$$V(r) = \frac{1}{2} \lambda^2 r^2 \quad (2.1)$$

where

$$r^2 = \sum_{j=1}^D x_j^2.$$

Thus the Schrödinger equation for the D -dimensional ($D \geq 2$) harmonic oscillator becomes

$$\left\{ -\frac{1}{2} \left(\frac{d^2}{dr^2} + \frac{(D-1)}{r} \frac{d}{dr} + \frac{\Lambda^2}{r^2} \right) + \frac{1}{2} \lambda^2 r^2 \right\} \psi_{n,l,\mu} = E_{n,l,\mu} \psi_{n,l,\mu}$$

with Λ^2 the non-radial part of the operator. Here n is the principal quantum number, l is the angular quantum number, and the μ_j are integers satisfying

$$l = \mu_1 \geq \mu_2 \geq \cdots \geq \mu_{D-1}$$

with $\mu_{D-1} = |m|$. It is known [5] that

$$\Lambda^2 Y_{l,\mu}(\Omega_D) = l(l+D-2)Y_{l,\mu}(\Omega_D)$$

where $Y_{l,\mu}(\Omega_D)$ are the hyperspherical harmonics defined by

$$Y_{l,\mu}(\Omega_D) = N_{l,\mu} e^{im\phi} \prod_{j=1}^{D-2} C_{\mu_j - \mu_{j+1}}^{\alpha_j + \mu_{j+1}}(\cos \theta_j) (\sin \theta_j)^{\mu_{j+1}} \quad (2.2)$$

with $N_{l,\mu}$ the normalization constant

$$N_{l,\mu}^{-2} = 2\pi \prod_{j=1}^{D-2} \frac{\sqrt{\pi} \Gamma(\alpha_j + \mu_{j+1} + \frac{1}{2})(\alpha_j + \mu_{j+1})(2\alpha_j + \mu_j + \mu_{j+1} - 1)!}{\Gamma(\alpha_j + \mu_{j+1} + 1)(\mu_j - \mu_{j+1})!(\alpha_j + \mu_j)(2\alpha_j + 2\mu_{j+1} - 1)!}.$$

Here $2\alpha_j = D - j - 1$, $C_n^\lambda(t)$ is the *Gegenbauer polynomial* of degree n and parameter λ and the angles $\theta_1, \theta_2, \dots, \theta_{D-2}, \phi$ are given by

$$\begin{aligned} x_1 &= r \sin \theta_1 \sin \theta_2 \cdots \sin \theta_{D-2} \cos \phi, \\ x_2 &= r \sin \theta_1 \sin \theta_2 \cdots \sin \theta_{D-2} \sin \phi, \\ x_3 &= r \sin \theta_1 \sin \theta_2 \cdots \cos \theta_{D-2}, \\ &\vdots \\ x_{D-1} &= r \sin \theta_1 \cos \theta_2, \\ x_D &= r \cos \theta_1, \end{aligned}$$

with $0 \leq \theta_j \leq \pi$ ($j = 1, 2, \dots, D-2$) and $0 \leq \phi < 2\pi$.

Separating variables by assuming the form of the wave function

$$\psi_{n,l,\mu} = R_{n,l}(r) Y_{l,\mu}(\Omega_D)$$

gives the equation

$$\left\{ -\frac{1}{2} \left(\frac{d^2}{dr^2} + \frac{(D-1)}{r} \frac{d}{dr} + \frac{l(l+D-2)}{r^2} \right) + \frac{1}{2} \lambda^2 r^2 \right\} R_{n,l} = E_{n,l} R_{n,l}.$$

With some substitutions and changes of variables, we then obtain the normalized solution

$$\psi_{n,l,\mu}(\vec{r}) = \left(\frac{2n! \lambda^{l+D/2}}{\Gamma(n+l+D/2)} \right)^{1/2} r^l e^{-\lambda r^2/2} L_n^{l-1+D/2}(\lambda r^2) Y_{l,\mu}(\Omega_D) \quad (2.3)$$

where $n = 0, 1, 2, \dots$ and $l = 0, 1, 2, \dots$, which corresponds with the energy

$$E_{n,l} = \lambda(2n + l + D/2).$$

If we take the Fourier transform of the wave function $\psi_{n,l,\mu}$, then we obtain the wave function in the momentum space

$$\hat{\psi}_{n,l,\mu}(\vec{p}) = (-1)^n \left(\frac{2n! \lambda^{-l-D/2}}{\Gamma(n+l+D/2)} \right)^{1/2} p^l e^{-p^2/2\lambda} L_n^{l-1+D/2}(p^2/\lambda) Y_{l,\mu}(\Omega_D). \quad (2.4)$$

Here and in the wave function $\psi_{n,l,\mu}$, we have used the *Laguerre polynomial* $L_n^\alpha(t)$.

3. The entropy for the harmonic oscillator

The densities in position space and momentum space are, respectively,

$$\rho(\vec{r}) = \frac{2n!\lambda^{l+D/2}}{\Gamma(n+l+D/2)} r^{2l} e^{-\lambda r^2} \left[L_n^{l-1+D/2}(\lambda r^2) \right]^2 |Y_{l,\mu}(\Omega_r)|^2, \quad (3.1)$$

$$\gamma(\vec{p}) = \frac{2n!\lambda^{-l-D/2}}{\Gamma(n+l+D/2)} p^{2l} e^{-p^2/\lambda} \left[L_n^{l-1+D/2}(p^2/\lambda) \right]^2 |Y_{l,\mu}(\Omega_p)|^2. \quad (3.2)$$

The information entropies in the position space and momentum space then are defined as

$$S_\rho = - \int \rho(\vec{r}) \log \rho(\vec{r}) d\vec{r}, \quad S_\gamma = - \int \gamma(\vec{p}) \log \gamma(\vec{p}) d\vec{p},$$

with

$$d\vec{r} = r^{D-1} dr d\Omega_D, \quad d\Omega_D = \left(\prod_{j=1}^{D-2} \sin^{2\alpha_j} \theta_j d\theta_j \right) d\phi.$$

For the D -dimensional ($D \geq 2$) harmonic oscillator we then obtain the following expressions for the entropies.

GROUND STATE: this is the state with the smallest energy ($E_{0,0} = \lambda D/2$)

$$\begin{aligned} S_\rho^0 &= -\frac{D}{2} \log \frac{\lambda}{\pi} + \frac{D}{2}, \\ S_\gamma^0 &= \frac{D}{2} \log \lambda \pi + \frac{D}{2}, \\ S_\rho^0 + S_\gamma^0 &= D(1 + \log \pi). \end{aligned}$$

ARBITRARY STATES: if the quantum numbers n, l, μ are arbitrary, then

$$\begin{aligned} S_\rho^{n,l,\mu} &= -\log \left(\frac{2n!}{\Gamma(n+l+D/2)} \right) - \frac{n!}{\Gamma(n+l+D/2)} (I_1 + I_2) \\ &\quad - I_3 + l + 2n + \frac{D}{2} - \frac{D}{2} \log \lambda \end{aligned} \quad (3.3)$$

and

$$\begin{aligned} S_\gamma^{n,l,\mu} &= -\log \left(\frac{2n!}{\Gamma(n+l+D/2)} \right) - \frac{n!}{\Gamma(n+l+D/2)} (I_1 + I_2) \\ &\quad - I_3 + l + 2n + \frac{D}{2} + \frac{D}{2} \log \lambda \end{aligned} \quad (3.4)$$

where

$$\begin{aligned} I_1 &= \int_0^\infty t^{l-1+D/2} e^{-t} \log t^l \left(L_n^{l-1+D/2}(t) \right)^2 dt, \\ I_2 &= \int_0^\infty t^{l-1+D/2} e^{-t} \left(L_n^{l-1+D/2}(t) \right)^2 \log \left(L_n^{l-1+D/2}(t) \right)^2 dt, \\ I_3 &= \int |Y_{l,\mu}(\Omega_D)|^2 \log |Y_{l,\mu}(\Omega_D)|^2 d\Omega_D. \end{aligned}$$

Consequently, we easily obtain

$$S_\rho^{n,l,\mu} + S_\gamma^{n,l,\mu} = -2 \log \left(\frac{2n!}{\Gamma(n+l+D/2)} \right) - \frac{2n!}{\Gamma(n+l+D/2)} (I_1 + I_2) - 2I_3 + 2l + 4n + D.$$

For the harmonic oscillator in one dimension, we only have one quantum number n and no angular part in the Schrödinger equation. The wave functions are now in terms of *Hermite polynomials*, and the corresponding densities are [7]

$$\rho(x) = \sqrt{\frac{\lambda}{\pi}} \frac{1}{2^n n!} e^{-\lambda x^2} H_n^2(x\sqrt{\lambda}), \tag{3.5}$$

$$\gamma(p) = \frac{1}{\sqrt{\lambda\pi} 2^n n!} e^{-p^2/\lambda} H_n^2(p/\sqrt{\lambda}). \tag{3.6}$$

For the ground state $n = 0$, we thus find

$$S_\rho^0 = \frac{1}{2} \log \pi + \frac{1}{2} - \frac{1}{2} \log \lambda,$$

$$S_\gamma^0 = \frac{1}{2} \log \pi + \frac{1}{2} + \frac{1}{2} \log \lambda,$$

and for the first excited state $n = 1$,

$$S_\rho^1 = -\frac{1}{2} \log \frac{4}{\pi} - \frac{1}{2} + C + 2 \log 2 - \frac{1}{2} \log \lambda,$$

$$S_\gamma^1 = -\frac{1}{2} \log \frac{4}{\pi} - \frac{1}{2} + C + 2 \log 2 + \frac{1}{2} \log \lambda$$

where $C = 0.5772156649\dots$ is Euler's constant. For arbitrary states n , we have

$$S_\rho^n = \log(\sqrt{\pi} 2^n n!) + n + \frac{1}{2} - (\sqrt{\pi} 2^n n!)^{-1} I_4 - \frac{1}{2} \log \lambda, \tag{3.7}$$

$$S_\gamma^n = \log(\sqrt{\pi} 2^n n!) + n + \frac{1}{2} - (\sqrt{\pi} 2^n n!)^{-1} I_4 + \frac{1}{2} \log \lambda \tag{3.8}$$

where

$$I_4 = \int_{-\infty}^{\infty} H_n^2(x) \log H_n^2(x) e^{-x^2} dx.$$

For the harmonic oscillator in two dimensions, we have two quantum numbers n and l . The ground state has the usual entropies, and the first excited state $n = 0, l = 1$ has the entropies

$$S_\rho^{0,1} = -\log \lambda + \log \pi + C + 1,$$

$$S_\gamma^{0,1} = \log \lambda + \log \pi + C + 1,$$

with C being Euler's constant. For arbitrary states n, l , the entropies involve the integrals I_1 and I_2 , given above, associated with the Laguerre polynomial $L_n^l(t)$.

Finally for the harmonic oscillator in three dimensions, we have three quantum numbers n, l, m . For the ground state, we have the usual simple expressions. The first

excited states $n = 0, l = 1$ have the entropies

$$\begin{aligned} S_\rho^{0,1,0} &= -\frac{3}{2} \log \lambda + \frac{3}{2} \log \pi + \log 2 + C + \frac{1}{2}, \\ S_\gamma^{0,1,0} &= \frac{3}{2} \log \lambda + \frac{3}{2} \log \pi + \log 2 + C + \frac{1}{2}, \\ S_\rho^{0,1,1} &= -\frac{3}{2} \log \lambda + \frac{3}{2} \log \pi + C + \frac{3}{2}, \\ S_\gamma^{0,1,1} &= \frac{3}{2} \log \lambda + \frac{3}{2} \log \pi + C + \frac{3}{2} \end{aligned}$$

where again C is Euler's constant. For arbitrary states, we need to take the integral I_3 into consideration. In three dimensions for $m \geq 0$, this integral is

$$\begin{aligned} I_3 &= \int |Y_{l,m}(\Omega_3)|^2 \log |Y_{l,m}(\Omega_3)|^2 d\Omega_3 \\ &= \log \left(\frac{(2l+1)(l-m)!}{4\pi(l+m)!} \right) + \left(\frac{(2l+1)(l-m)!}{2(l+m)!} \right) \int_{-1}^1 [P_l^m(t)]^2 \log [P_l^m(t)]^2 dt \end{aligned}$$

where $P_l^m(t)$ are Legendre functions. If we use the relationship with Gegenbauer polynomials

$$(-1)^m \frac{(1-t^2)^{-m/2} m! 2^m}{(2m)!} P_l^m(t) = C_{l-m}^{m+1/2}(t),$$

this integral becomes

$$I_3 = \log \left(\frac{(2l+1)(l-m)!}{4\pi(l+m)!} \right) + \left(\frac{(2l+1)(l-m)! [(2m)!]^2}{2^{2m+1}(l+m)!(m!)^2} \right) (I_5 + I_6) + 2 \log \left(\frac{(2m)!}{m! 2^m} \right)$$

with

$$\begin{aligned} I_5 &= \int_{-1}^1 [C_{l-m}^{m+1/2}(t)]^2 (1-t^2)^m \log(1-t^2)^m dt, \\ I_6 &= \int_{-1}^1 [C_{l-m}^{m+1/2}(t)]^2 (1-t^2)^m \log [C_{l-m}^{m+1/2}(t)]^2 dt. \end{aligned}$$

In the case that $m < 0$, it suffices [7] to substitute m for $|m|$.

4. The hydrogen atom

The usual way to describe the hydrogen atom is by means of the radially symmetric Coulomb potential

$$V(r) = -\frac{1}{r}, \quad r^2 = \sum_{i=1}^D x_i^2. \quad (4.1)$$

The wave functions in position space are given in atomic units [13] by

$$\psi(\vec{r}) = N_{n,l} e^{-r/2\lambda} (r/\lambda)^l L_{n-l-1}^{2l+D-2}(r/\lambda) Y_{l,\mu}(\Omega_D) \quad (4.2)$$

where $N_{n,l}$ are normalizing constants given by

$$N_{n,l} = \lambda^{-D/2} \left(\frac{(n-l-1)!}{2^n (n+l+D-3)!} \right)^{1/2}$$

with

$$\eta = n + \frac{D-3}{2}, \quad \lambda = \frac{\eta}{2}.$$

The quantum numbers $n = 1, 2, 3, \dots$ and $l = 0, 1, \dots, n-1$ correspond to the energy

$$E_n = \frac{-1}{2\eta^2}.$$

The associated probability density then is

$$\rho(\vec{r}) = |\psi(\vec{r})|^2 = N_{n,l}^2 e^{-r/\lambda} (r/\lambda)^{2l} [L_{n-l-1}^{2l+D-2}(r/\lambda)]^2 |Y_{l,\mu}(\Omega_D)|^2. \quad (4.3)$$

By using a generalization of the method used by Fock [5], we find that the wave function in momentum space is

$$\hat{\psi}(\vec{p}) = \frac{(2p_0)^{1+D/2}}{\sqrt{2}(p_0^2 + p^2)^{(D+1)/2}} Y_{n-1,l,\mu}(\Omega_{D+1})$$

where $p_0^2 = -2E_n = \eta^{-2}$. If we use the known relationship between the hyperspherical harmonics in a $(D+1)$ -dimensional space and those in a D -dimensional space, the wave function also is equal to

$$\hat{\psi}(\vec{p}) = K_{n,l} \frac{(\eta p)^l}{(1 + \eta^2 p^2)^{l+(D+1)/2}} C_{n-l-1}^{l+(D-1)/2} \left(\frac{1 - \eta^2 p^2}{1 + \eta^2 p^2} \right) Y_{l,\mu}(\Omega_D) \quad (4.4)$$

where $C_n^\alpha(t)$ is a Gegenbauer polynomial, η has the same meaning as in the position space, and

$$K_{n,l} = \left(\frac{(n-l-1)!}{2\pi(n+l+D-3)!} \right)^{1/2} 2^{2l+D} \Gamma\left(1 + \frac{D-1}{2}\right) \eta^{(D+1)/2}.$$

With this the corresponding density becomes

$$\gamma(\vec{p}) = |\hat{\psi}(\vec{p})|^2 = K_{n,l}^2 \frac{(\eta p)^{2l}}{(1 + \eta^2 p^2)^{2l+D+1}} \left[C_{n-l-1}^{l+(D-1)/2} \left(\frac{1 - \eta^2 p^2}{1 + \eta^2 p^2} \right) \right]^2 |Y_{l,\mu}(\Omega_D)|^2. \quad (4.5)$$

5. The entropy for the hydrogen atom

The information entropy in position space thus becomes

$$\begin{aligned} S_\rho &= - \int \rho(\vec{r}) \log \rho(\vec{r}) d\vec{r} \\ &= - \log N_{n,l}^2 + \lambda^D N_{n,l}^2 (J_1 - 2lJ_2 - J_3) - J_4 \end{aligned} \quad (5.1)$$

where

$$\begin{aligned} J_1 &= \frac{(n+l+D-1)!}{(n-l-1)!} + 4 \frac{(n+l+D-2)!}{(n-l-2)!} + \frac{(n+l+D-3)!}{(n-l-3)!}, \\ J_2 &= \int_0^\infty t^{\alpha+1} e^{-t} \log t [L_k^\alpha(t)]^2 dt, \\ J_3 &= \int_0^\infty t^{\alpha+1} e^{-t} [L_k^\alpha(t)]^2 \log [L_k^\alpha(t)]^2 dt, \\ J_4 &= \int |Y_{l,\mu}(\Omega_D)|^2 \log |Y_{l,\mu}(\Omega_D)|^2 d\Omega_D, \end{aligned}$$

with $k = n - l - 1$ and $\alpha = 2l + D - 2$. In momentum space, we find

$$\begin{aligned} S_\gamma &= - \int \gamma(\vec{p}) \log \gamma(\vec{p}) d\vec{p} \\ &= - \log K_{n,l}^2 + (2l + D + 1) \log 2 - \frac{K_{n,l}^2}{\eta^D 2^{2l+D+1}} [lJ_5 + (D + 1)J_6 + J_7] - J_4 \end{aligned} \quad (5.2)$$

where

$$\begin{aligned} J_5 &= \int_{-1}^1 (1 - t^2)^{\nu-1/2} \log(1 - t^2) [C_k^\nu(t)]^2 dt, \\ J_6 &= \int_{-1}^1 (1 - t^2)^{\nu-1/2} (1 + t) \log(1 + t) [C_k^\nu(t)]^2 dt, \\ J_7 &= \int_{-1}^1 (1 - t^2)^{\nu-1/2} [C_k^\nu(t)]^2 \log [C_k^\nu(t)]^2, \end{aligned}$$

with $k = n - l - 1$ and $\nu = l + (D - 1)/2$.

For the Coulomb potential in one dimension, we have

$$V(x) = -\frac{1}{|x|}. \quad (5.3)$$

The ground state has a degenerate energy $E_0 = -\infty$, and thus some care has to be taken in analysing this state. The wave function in position space is most appropriately given [11] by

$$\psi(x) = \alpha^{-1/2} e^{-|x|/\alpha}, \quad \alpha \rightarrow 0. \quad (5.4)$$

By taking the Fourier transform, we obtain the wave function in the momentum space

$$\hat{\psi}(p) = \sqrt{\frac{2}{\pi}} \frac{\alpha^{1/2}}{1 + \alpha^2 p^2}, \quad \alpha \rightarrow 0. \quad (5.5)$$

The entropies for $\alpha > 0$ thus are given by

$$S_\rho = 1 + \log \alpha, \quad S_\gamma = -\log \alpha + \log \frac{\pi}{2} + 4 \log 2 - 2; \quad (5.6)$$

hence

$$S_\rho + S_\gamma = \log \frac{\pi}{2} + 4 \log 2 - 1,$$

independent of α . The wave functions for the other states are [11]

$$\psi_{\text{even}}(x) = \sqrt{\frac{2}{n^5}} e^{-|x|/n} |x| L_{n-1}^1(2|x|/n), \quad (5.7)$$

$$\psi_{\text{odd}}(x) = \sqrt{\frac{2}{n^5}} e^{-|x|/n} x L_{n-1}^1(2|x|/n) \quad (5.8)$$

where $\psi_{\text{even}}(x)$ is the wave function for even states and $\psi_{\text{odd}}(x)$ for odd states. In momentum space, the wave functions are [8]

$$\hat{\psi}(p) = \sqrt{\frac{2}{\pi}} \frac{\sqrt{ne}^{\pm 2in \arctan(np)}}{1 + n^2 p^2} \quad (5.9)$$

with $n = 1, 2, 3, \dots$. The state n has the energy $E_n = -1/n^2$. The densities in position and momentum space thus are

$$\rho(x) = \frac{2}{n^5} e^{-2|x|/n} x^2 [L_{n-1}^1(2|x|/n)]^2, \tag{5.10}$$

$$\gamma(p) = \frac{2}{\pi} \frac{n}{(1 + n^2 p^2)^2}, \tag{5.11}$$

with corresponding entropies

$$S_\rho = 3 \log n + \log 2 + 3n - \frac{1}{n^2} (J_2 + J_3/2), \tag{5.12}$$

$$S_\gamma = \log \pi - \log n + 3 \log 2 - 2 \tag{5.13}$$

where

$$J_2 = \int_0^\infty t^2 e^{-t} \log t [L_{n-1}^1(t)]^2 dt,$$

$$J_3 = \int_0^\infty t^2 e^{-t} [L_{n-1}^1(t)]^2 \log [L_{n-1}^1(t)]^2 dt.$$

The entropies for the Coulomb potential in two and three dimensions easily can be obtained from the general expressions obtained above by putting $D = 2$ and $D = 3$, respectively.

6. Entropy for orthogonal polynomials

From the previous sections, we see that the information entropies S_ρ and S_γ for the harmonic oscillator and the Coulomb potential are in terms of entropy integrals of the form

$$E_n = \int p_n^2(x) \log p_n^2(x) d\mu(x) \tag{6.1}$$

where p_n ($n = 0, 1, 2, 3, \dots$) are orthogonal polynomials with respect to a positive measure μ on the real line. The polynomials of interest are the Gegenbauer polynomials (for I_6 and J_7), the Laguerre polynomials (for I_2 and J_3), and the Hermite polynomials (for I_4). In a more general setting, we will study, in the remainder of this section, entropy integrals of the form (6.1) for orthogonal polynomials on the real line. In the next section, we will restrict attention to the Gegenbauer polynomials. In Section 8, the Laguerre and the Hermite polynomials are treated.

If p_n ($n = 0, 1, 2, \dots$) are orthogonal polynomials on the real line, then their zeros $x_{j,n}$ ($j = 1, 2, \dots, n$) are all real and simple. We then can write $p_n(x) = k_n \prod_{j=1}^n (x - x_{j,n})$, with k_n the leading coefficient of p_n , to find

$$\log p_n^2(x) = 2 \log k_n + 2 \sum_{j=1}^n \log |x - x_{j,n}|,$$

so that

$$E_n = 2 \log k_n \int p_n^2(x) d\mu(x) + 2 \sum_{j=1}^n \int p_n^2(x) \log |x - x_{j,n}| d\mu(x).$$

If μ is a probability measure, then

$$U(z; \mu) = \int \log \frac{1}{|z-x|} d\mu(x)$$

is known as the *logarithmic potential* of the measure μ [14, p. 164]. Consider the zero distribution for p_n , i.e., the discrete measure

$$\mu_n = \frac{1}{n} \sum_{j=1}^n \delta(x - x_{j,n})$$

which has mass $1/n$ at each zero of p_n . Obviously $\log |p_n(z)| = \log k_n - nU(z; \mu_n)$. If the polynomials are orthonormal, then the leading coefficient usually is denoted by γ_n , and we then have

$$E_n = 2 \log \gamma_n - 2n \int U(x; \mu_n) p_n^2(x) d\mu(x). \quad (6.2)$$

The double integral

$$I(\mu, \nu) = \iint \log \frac{1}{|x-y|} d\mu(x) d\nu(y)$$

is known as the *mutual energy* of the two measures μ and ν [14, p. 168], and when $\mu = \nu$, then $I(\mu, \mu) = I(\mu)$ is the (logarithmic) energy of μ . If we define for the orthonormal polynomial p_n the probability measure ν_n by

$$d\nu_n(x) = p_n^2(x) d\mu(x),$$

then this gives us a relation between the mutual energy of μ_n and ν_n and the entropy E_n :

$$E_n = 2 \log \gamma_n - 2nI(\mu_n, \nu_n). \quad (6.3)$$

The two measures give interesting information about the polynomial p_n and its zeros; in particular, μ_n has all its mass in the neighbourhood of the zeros of p_n , whereas ν_n has little mass in the neighborhood of the zeros.

For a large class of orthogonal polynomials (the class $M(1, 0)$ defined in [12]), it is known that both measures μ_n and ν_n converge weakly to the measure μ_0 given by

$$d\mu_0(x) = \frac{1}{\pi} \frac{dx}{\sqrt{1-x^2}}, \quad -1 < x < 1,$$

[16, Thm. 2] and that $\lim_{n \rightarrow \infty} \gamma_n^{1/n} = 2$; hence for orthonormal polynomials in $M(1, 0)$, such as the Jacobi polynomials, one expects $E_n \sim 2n \log 2 - 2nI(\mu_0)$, and since $I(\mu_0) = \log 2$, this gives $E_n/n \rightarrow 0$ and indicates that the terms $2 \log \gamma_n$ and $2nI(\mu_n, \nu_n)$ are of the same order.

By using Fubini's theorem, we can write (6.2) or (6.3) as

$$E_n = 2 \log \gamma_n - 2 \sum_{j=1}^n U(x_{j,n}; \nu_n), \quad (6.4)$$

which is in terms of the logarithmic potential

$$U(z; \nu_n) = \int p_n^2(x) \log \frac{1}{|z-x|} d\mu(x) \quad (6.5)$$

of the measure ν_n . If we restrict attention to the case where the measure μ is supported on the interval $[-1, 1]$, then μ_0 can be identified with the equilibrium measure on $[-1, 1]$ which minimizes the energy $I(\mu)$ over all probability measures supported on $[-1, 1]$. The logarithmic potential $U(z; \mu_0)$ is the constant equal to $\log 2$ on $[-1, 1]$ [17, §1.1 and 1.3]. Furthermore, for any other measures on $[-1, 1]$, one has

$$\min_{z \in [-1, 1]} U(z; \mu) \leq I(\mu_0) = \log 2 \leq \max_{z \in [-1, 1]} U(z; \mu),$$

which shows that $U(z; \nu_n)$ oscillates around $\log 2$ for $z \in [-1, 1]$. To find the extrema, we consider

$$\frac{d}{dz} U(z; \nu_n) = \frac{d}{dz} \int_{-1}^1 p_n^2(x) \log \frac{1}{|z-x|} d\mu(x) = \int_{-1}^1 \frac{p_n^2(x)}{x-z} d\mu(x).$$

For $z \in (-1, 1)$, this integral must be considered as a Cauchy principal value integral. It can be written as

$$\int_{-1}^1 \frac{p_n^2(x)}{x-z} d\mu(x) = \int_{-1}^1 p_n(x) \frac{p_n(x) - p_n(z)}{x-z} d\mu(x) + p_n(z) \int_{-1}^1 \frac{p_n(x)}{x-z} d\mu(x).$$

Now $[p_n(x) - p_n(z)]/(x-z)$ is a polynomial in x of degree less than n ; hence by orthogonality

$$\int_{-1}^1 \frac{p_n^2(x)}{x-z} d\mu(x) = -p_n(z)q_n(z)$$

where $q_n(z) = \int p_n(x)/(z-x) d\mu(x)$ is the function of the second kind [17, p. 159]. It follows that the extrema of $U(z; \nu_n)$ are given by the zeros of p_n and q_n . To see whether we are dealing with minima or maxima, we consider the second derivative

$$\frac{d^2}{dz^2} U(z; \nu_n) = -p'_n(z)q_n(z) - p_n(z)q'_n(z),$$

and at the zeros of p_n , this gives

$$\frac{d^2}{dz^2} U(x_{j,n}; \nu_n) = -p'_n(x_{j,n})q_n(x_{j,n}).$$

Consider the associated polynomials

$$p_{n-1}^{(1)}(z) = \int \frac{p_n(z) - p_n(x)}{z-x} d\mu(x) = p_n(z)q_0(z) - q_n(z).$$

Then at the zeros of p_n , this gives $p_{n-1}^{(1)}(x_{j,n}) = -q_n(x_{j,n})$, so that $-p'_n(x_{j,n})q_n(x_{j,n}) = p_{n-1}^{(1)}(x_{j,n})p'_n(x_{j,n})$, and this is a positive quantity because the zeros of p_n and $p_{n-1}^{(1)}$ interlace. Hence, the zeros of p_n are all local minima for $U(z; \nu_n)$. This means, by formula (6.4), that in order to compute E_n we need to take a sum of the logarithmic potential $U(z; \nu_n)$ evaluated at its local minima. For this reason, we will investigate the logarithmic potential $U(z; \nu_n)$ in detail for Gegenbauer polynomials (Section 7) and for Laguerre and Hermite polynomials (Section 8).

7. Logarithmic potentials for Gegenbauer polynomials

Gegenbauer polynomials (ultraspherical polynomials) are symmetric Jacobi polynomials. They are denoted by $C_n^\lambda(x)$, with $\lambda > -1/2$ and satisfy the orthogonality [15, §4.7]

$$\frac{1}{\pi} \int_{-1}^1 C_n^\lambda(x) C_m^\lambda(x) (1-x^2)^{\lambda-\frac{1}{2}} dx = \frac{2^{1-2\lambda} \Gamma(n+2\lambda)}{\Gamma^2(\lambda)(n+\lambda)n!} \delta_{m,n}. \quad (7.1)$$

Observe that the polynomials C_n^λ are not orthonormal, and that the orthogonality measure is not yet normalized to a probability measure.

Gegenbauer polynomials have some useful properties, and by differentiation, one can go from polynomials with parameter λ to polynomials with parameter $\lambda \pm 1$. To go from λ to $\lambda + 1$, one uses

$$(C_n^\lambda(x))' = 2\lambda C_{n-1}^{\lambda+1}(x), \quad (7.2)$$

and to go from λ to $\lambda - 1$, we can use

$$(1-x^2)^{\lambda-\frac{1}{2}} C_n^\lambda(x) = -\frac{2\lambda}{(2\lambda+n)n} \left((1-x^2)^{\lambda+\frac{1}{2}} C_{n-1}^{\lambda+1}(x) \right)', \quad (7.3)$$

which follows from Rodrigues' formula. If we want to use probability measures, then we use

$$\int_{-1}^1 (1-x^2)^{\lambda-\frac{1}{2}} dx = \frac{\sqrt{\pi} \Gamma(\lambda + \frac{1}{2})}{\Gamma(\lambda + 1)},$$

so that

$$w_\lambda(x) = \frac{\Gamma(\lambda + 1)}{\sqrt{\pi} \Gamma(\lambda + \frac{1}{2})} (1-x^2)^{\lambda-\frac{1}{2}} \quad (7.4)$$

is a probability density on $[-1, 1]$. The orthonormal polynomials for this probability measure are given by

$$p_n^\lambda(x) = \left(\frac{n+\lambda}{\lambda} \frac{\Gamma(2\lambda)}{\Gamma(n+2\lambda)} n! \right)^{1/2} C_n^\lambda(x), \quad (7.5)$$

and thus

$$\int_{-1}^1 p_n^\lambda(x) p_m^\lambda(x) w_\lambda(x) dx = \delta_{m,n}.$$

Since the weight function is symmetric, it follows that the Gegenbauer polynomials of even degree are even functions, whereas the Gegenbauer polynomials of odd degree are odd functions. Finally, from

$$C_n^\lambda(x) = \frac{2^n \Gamma(n+\lambda)}{n! \Gamma(\lambda)} x^n + \dots, \quad (7.6)$$

one can immediately read off the leading coefficient.

In this section, our interest is the logarithmic potential

$$V_n^\lambda(t) = - \int_{-1}^1 [C_n^\lambda(x)]^2 \log|x-t| (1-x^2)^{\lambda-\frac{1}{2}} dx, \quad (7.7)$$

which is related to the logarithmic potential $U(t; \nu_n)$, defined in (6.5), by

$$\begin{aligned} U(t; \nu_n) &:= \hat{V}_n^\lambda(t) = \frac{n + \lambda}{\lambda} \frac{\Gamma(2\lambda)}{\Gamma(n + 2\lambda)} \frac{n! \Gamma(\lambda + 1)}{\sqrt{\pi} \Gamma(\lambda + \frac{1}{2})} V_n^\lambda(t) \\ &= - \int_{-1}^1 [p_n^\lambda(x)]^2 \log |x - t| w_\lambda(x) dx. \end{aligned}$$

Taking into account that the leading coefficient of the orthonormal polynomial p_n^λ is

$$\gamma_n = \frac{2^n \Gamma(\lambda + n + 1) \Gamma(2\lambda)}{\Gamma(\lambda + 1) \Gamma(n + 2\lambda)}, \tag{7.8}$$

a precise knowledge of the function V_n^λ at the zeros of C_n^λ would allow us to compute the entropy for Gegenbauer polynomials by means of (6.4).

Let us first consider the special cases $\lambda = 0$ and $\lambda = 1$. For $\lambda \rightarrow 0$, we have

$$\lim_{\lambda \rightarrow 0} \frac{1}{\lambda} C_n^\lambda(x) = \frac{2}{n} T_n(x), \quad n \neq 0$$

where T_n are the Chebyshev polynomials of the first kind. For $\lambda = 1$ we have

$$C_n^1(x) = U_n(x),$$

where U_n are the Chebyshev polynomials of the second kind. If $x, t \in [-1, 1]$, then one can find $\theta, \phi \in [0, \pi]$ such that $x = \cos \phi$ and $t = \cos \theta$. One then has

$$\begin{aligned} |x - t| &= |\cos \phi - \cos \theta| \\ &= \frac{1}{2} |e^{i\phi} + e^{-i\phi} - e^{i\theta} - e^{-i\theta}| \\ &= \frac{1}{2} |e^{i\phi} - e^{i\theta}| |e^{i\phi} - e^{-i\theta}|. \end{aligned}$$

Therefore,

$$\log |x - t| = \log \frac{1}{2} + \log |e^{i\phi} - e^{i\theta}| + \log |e^{i\phi} - e^{-i\theta}|.$$

Use the Fourier series [10, p. 38]

$$\sum_{k=1}^{\infty} \frac{\cos k\varphi}{k} = -\log |1 - e^{i\varphi}|, \quad 0 < \varphi < 2\pi,$$

to find that, for $x \neq t$,

$$\begin{aligned} \log |x - t| &= \log \frac{1}{2} - \sum_{k=1}^{\infty} \frac{\cos k(\phi - \theta)}{k} - \sum_{k=1}^{\infty} \frac{\cos k(\phi + \theta)}{k} \\ &= \log \frac{1}{2} - 2 \sum_{k=1}^{\infty} \frac{1}{k} T_k(x) T_k(t). \end{aligned} \tag{7.9}$$

If we set

$$\hat{V}_n^0(t) = \lim_{\lambda \rightarrow 0} \frac{n^2}{2\pi\lambda^2} V_n^\lambda(t) = -\frac{2}{\pi} \int_{-1}^1 T_n^2(x) \log |x - t| \frac{dx}{\sqrt{1 - x^2}},$$

then by (7.9), we have for $-1 < t < 1$

$$\hat{V}_n^0(t) = \log 2 \frac{2}{\pi} \int_{-1}^1 T_n^2(x) \frac{dx}{\sqrt{1-x^2}} + 2 \sum_{j=1}^{\infty} \frac{T_j}{j} \frac{2}{\pi} \int_{-1}^1 T_n^2(x) T_j(x) \frac{dx}{\sqrt{1-x^2}}.$$

Using simple trigonometry and $T_n(x) = \cos n\theta$ for $x = \cos \theta$, we have

$$T_n^2(x) = \frac{1}{2} [T_{2n}(x) + 1],$$

and by the orthogonality of the Chebyshev polynomials of the first kind

$$\frac{2}{\pi} \int_{-1}^1 T_n(x) T_m(x) \frac{dx}{\sqrt{1-x^2}} = \delta_{m,n}, \quad n, m \geq 1.$$

This gives

$$\frac{2}{\pi} \int_{-1}^1 T_n^2(x) T_j(x) \frac{dx}{\sqrt{1-x^2}} = \frac{1}{4} \delta_{j,2n},$$

so that

$$\hat{V}_n^0(t) = \log 2 + \frac{T_{2n}(t)}{2n}, \quad -1 < t < 1, \quad n \geq 1. \quad (7.10)$$

In a similar way, we have for $\lambda = 1$

$$\hat{V}_n^1(t) = \frac{2}{\pi} V_n^1(t) = -\frac{2}{\pi} \int_{-1}^1 U_n^2(x) \sqrt{1-x^2} \log|x-t| dx,$$

and if we use

$$T_{n+1}^2(x) + (1-x^2)U_n^2(x) = 1, \quad (7.11)$$

then this gives

$$\begin{aligned} \hat{V}_n^1(t) &= -\frac{2}{\pi} \int_{-1}^1 [1 - T_{n+1}^2(x)] \log|x-t| \frac{dx}{\sqrt{1-x^2}} \\ &= 2 \log 2 - \hat{V}_{n+1}^0(t), \end{aligned}$$

so that

$$\hat{V}_n^1(t) = \log 2 - \frac{T_{2n+2}(t)}{2n+2}, \quad -1 < t < 1, \quad n \geq 0. \quad (7.12)$$

Observe that (7.10) and (7.12) indeed show that these logarithmic potentials oscillate around the value $\log 2$ when $t \in [-1, 1]$, as was explained in the previous section.

For other values of the parameter λ , the computation becomes more complicated. There is, however, an interesting extension of Euler's identity (7.11) for Gegenbauer polynomials, which was obtained by Dette [9, p.570]:

$$\left[\frac{n}{2\lambda} C_n^\lambda(x) \right]^2 + (1-x^2) [C_{n-1}^{\lambda+1}(x)]^2 = \sum_{j=0}^{n-1} \frac{j+\lambda}{\lambda} [C_j^\lambda(x)]^2. \quad (7.13)$$

If we multiply both sides of this identity by $(1 - x^2)^{\lambda - \frac{1}{2}} \log |x - t|$ and then integrate over $[-1, 1]$, then we obtain

$$\left(\frac{n}{2\lambda}\right)^2 V_n^\lambda(t) + V_{n-1}^{\lambda+1}(t) = \sum_{j=0}^{n-1} \frac{j + \lambda}{\lambda} V_j^\lambda(t). \tag{7.14}$$

This is a linear recurrence relation which allows the computation of the logarithmic potential $V_{n-1}^{\lambda+1}(t)$ whenever $V_0^\lambda, V_1^\lambda, \dots, V_n^\lambda$ are known. In particular, this recurrence allows us to obtain the logarithmic potentials $V_n^\lambda(t)$ for integer values of the parameter λ by using the explicit formulas (7.10) and (7.12) for the Chebyshev polynomials. A closed expression is not easily obtained, but the recurrence can be used effectively if λ is not large. For $\lambda = 2$, this gives

$$\hat{V}_n^2(t) = \log 2 + \frac{n + 1}{n + 3} \frac{T_{2n+4}(t)}{2n + 4} - \frac{U_{2n+2}(t)}{(n + 1)(n + 3)} + \frac{1}{(n + 1)(n + 3)}. \tag{7.15}$$

Observe that since $|T_n(t)| \leq 1$ and $|U_n(t)| \leq n + 1$ for every $t \in [-1, 1]$, we have $\hat{V}_n^2(t) = \log 2 + O(1/n)$ uniformly on $[-1, 1]$.

For the entropy E_n^λ , we need to evaluate the logarithmic potential at the zeros of the Gegenbauer polynomial C_n^λ . For the Chebyshev polynomials, we have that $T_n(x_{j,n}) = 0$ implies $T_{2n}(x_{j,n}) = -1$, so that $\hat{V}_n^0(x_{j,n}) = \log 2 - \frac{1}{2n}$. The entropy, given by (6.4), therefore is equal to

$$E_n^0 = 1 - \log 2, \quad n \geq 1,$$

confirming our result in [19]. For Chebyshev polynomials of the second kind, we have that $U_n(x_{j,n}) = 0$ implies $T_{2n+2}(x_{j,n}) = 1$, so that $\hat{V}_n^1(x_{j,n}) = \log 2 - \frac{1}{2n+2}$. By using (6.4), this then gives for the entropy

$$E_n^1 = \frac{n}{n + 1},$$

also confirming our result in [19].

The recurrence (7.14) still can be simplified. By using (7.3), we find

$$\begin{aligned} & \int_{-1}^1 [C_n^\lambda(x)]^2 \log |x - t| (1 - x^2)^{\lambda - \frac{1}{2}} dx \\ &= -\frac{2\lambda}{n(2\lambda + n)} \int_{-1}^1 C_n^\lambda(x) \log |x - t| d((1 - x^2)^{\lambda + \frac{1}{2}} C_{n-1}^{\lambda+1}(x)). \end{aligned}$$

Integration by parts and (7.2) then give

$$\begin{aligned} & \int_{-1}^1 [C_n^\lambda(x)]^2 \log |x - t| (1 - x^2)^{\lambda - \frac{1}{2}} dx \\ &= \frac{2\lambda}{(2\lambda + n)n} \int_{-1}^1 \frac{C_{n-1}^{\lambda+1}(x) C_n^\lambda(x)}{x - t} (1 - x^2)^{\lambda + \frac{1}{2}} dx \\ & \quad + \frac{(2\lambda)^2}{(2\lambda + n)n} \int_{-1}^1 [C_{n-1}^{\lambda+1}(x)]^2 \log |x - t| (1 - x^2)^{\lambda + \frac{1}{2}} dx. \end{aligned}$$

The first term on the right-hand side can be computed since by (7.6)

$$\frac{C_n^\lambda(x) - C_n^\lambda(t)}{x - t} = \frac{2\lambda}{n} C_{n-1}^{\lambda+1}(x) + g_{n-2}(x)$$

where g_{n-2} is some polynomial of degree at most $n - 2$, and thus by (7.1)

$$\begin{aligned} & \int_{-1}^1 \frac{C_{n-1}^{\lambda+1}(x)C_n^\lambda(x)}{x-t}(1-x^2)^{\lambda+\frac{1}{2}} dx \\ &= \frac{2\lambda}{n} \int_{-1}^1 [C_{n-1}^{\lambda+1}(x)]^2 (1-x^2)^{\lambda+\frac{1}{2}} dx - C_n^\lambda(t)Q_{n-1}^{\lambda+1}(t) \end{aligned}$$

where

$$Q_n^\lambda(t) = \int_{-1}^1 \frac{C_n^\lambda(x)}{t-x}(1-x^2)^{\lambda-\frac{1}{2}} dx$$

is the Gegenbauer function of the second kind. This means that

$$V_n^\lambda(t) = \frac{(2\lambda)^2}{(2\lambda+n)n} V_{n-1}^{\lambda+1}(t) + \frac{2\lambda}{(2\lambda+n)n} Q_{n-1}^{\lambda+1}(t)C_n^\lambda(t) - \frac{2\pi\Gamma(n+2\lambda)}{2^{2\lambda}n(n+\lambda)\Gamma^2(\lambda)n!}. \quad (7.16)$$

For the normalized potential \hat{V}_n^λ , this recurrence is

$$\hat{V}_n^\lambda(t) = \hat{V}_{n-1}^{\lambda+1}(t) - \frac{1}{n} + \frac{2(n+\lambda)\Gamma(2\lambda)(n-1)!\Gamma(\lambda+1)}{\sqrt{\pi}\Gamma(n+2\lambda+1)\Gamma(\lambda+1/2)} C_n^\lambda(t)Q_{n-1}^{\lambda+1}(t).$$

If we use (7.16) in (7.14), then we can eliminate $V_{n-1}^{\lambda+1}(t)$ and obtain a recurrence relation for $V_n^\lambda(t)$. This gives

$$n(n+\lambda)V_n^\lambda(t) = \lambda Q_{n-1}^{\lambda+1}(t)C_n^\lambda(t) - \frac{\pi\Gamma(n+2\lambda+1)}{2^{2\lambda}(n+\lambda)\Gamma^2(\lambda)n!} + 2\lambda^2 \sum_{j=0}^{n-1} \frac{j+\lambda}{\lambda} V_j^\lambda(t).$$

We can get rid of the sum on the right-hand side by taking the first difference on each side of the equation, giving

$$\begin{aligned} n(n+\lambda)V_n^\lambda(t) &= (\lambda+n-1)(2\lambda+n-1)V_{n-1}^\lambda(t) \\ &+ \lambda [Q_{n-1}^{\lambda+1}(t)C_n^\lambda(t) - Q_{n-2}^{\lambda+1}(t)C_{n-1}^\lambda(t)] - \frac{\pi\Gamma(n+2\lambda)}{2^{2\lambda}\Gamma^2(\lambda)n!} \left(\frac{n+2\lambda}{n+\lambda} - \frac{n}{n+\lambda-1} \right). \end{aligned} \quad (7.17)$$

This is a non-homogeneous first-order recurrence relation. The general solution of the homogeneous equation is

$$A \frac{(2\lambda)_n}{(n+\lambda)n!}$$

where A is independent of n . If we look for a solution of the form

$$V_n^\lambda(t) = A_n(t) \frac{(2\lambda)_n}{(n+\lambda)n!},$$

then

$$\begin{aligned} V_n^\lambda(t) &= \frac{\lambda(2\lambda)_n}{(n+\lambda)n!} \left(V_0^\lambda(t) + \sum_{k=1}^n \frac{(k-1)!}{(2\lambda)_k} [Q_{k-1}^{\lambda+1}(t)C_k^\lambda(t) - Q_{k-2}^{\lambda+1}(t)C_{k-1}^\lambda(t)] \right. \\ &\quad \left. - \frac{\pi\Gamma(2\lambda)}{2^{2\lambda}\lambda\Gamma^2(\lambda)} \left(\frac{1}{n+\lambda} - \frac{1}{\lambda} + 2\lambda \sum_{k=1}^n \frac{1}{k(k+\lambda)} \right) \right). \end{aligned}$$

8. Logarithmic potentials for Hermite and Laguerre polynomials

In a similar way, one can obtain recursive formulas for the logarithmic potentials involving squares of Hermite and Laguerre polynomials. For Hermite polynomials, we define

$$V_n(t) = - \int_{-\infty}^{\infty} H_n^2(x) \log|x-t| e^{-x^2} dx.$$

Recall that [15, p. 106]

$$H'_n(x) = 2nH_{n-1}(x), \tag{8.1}$$

and from Rodrigues's formula, we also have

$$(e^{-x^2} H_{n-1}(x))' = -e^{-x^2} H_n(x); \tag{8.2}$$

hence using (8.2), we have

$$V_n(t) = \int_{-\infty}^{\infty} H_n(x) \log|x-t| d(e^{-x^2} H_{n-1}(x)).$$

Now use integration by parts and (8.1) to find

$$V_n(t) = 2nV_{n-1}(t) - \int_{-\infty}^{\infty} e^{-x^2} \frac{H_n(x)H_{n-1}(x)}{x-t} dx.$$

The last integral can be written as

$$\begin{aligned} \int_{-\infty}^{\infty} e^{-x^2} \frac{H_n(x)H_{n-1}(x)}{x-t} dx &= \int_{-\infty}^{\infty} e^{-x^2} H_n(x) \frac{H_{n-1}(x) - H_{n-1}(t)}{x-t} dx \\ &\quad + H_{n-1}(t) \int_{-\infty}^{\infty} e^{-x^2} \frac{H_n(x)}{x-t} dx, \end{aligned}$$

and by orthogonality, we thus have

$$\int_{-\infty}^{\infty} e^{-x^2} \frac{H_n(x)H_{n-1}(x)}{x-t} dx = -H_{n-1}(t)Q_n(t)$$

where $Q_n(t)$ is the Hermite function of the second kind

$$Q_n(t) = \int_{-\infty}^{\infty} e^{-x^2} \frac{H_n(x)}{t-x} dx.$$

This gives the recursion

$$V_n(t) = 2nV_{n-1}(t) + H_{n-1}(t)Q_n(t). \tag{8.3}$$

For the normalized weight function $w(x) = \pi^{-1/2}e^{-x^2}$, the orthonormal Hermite polynomials are $p_n(x) = (2^n n!)^{-1/2}H_n(x)$, so that for the normalized potential, we have

$$\hat{V}_n(t) := -\frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-x^2} p_n^2(x) \log|x-t| dx = \frac{1}{2^n n! \sqrt{\pi}} V_n(t),$$

and the recurrence relation becomes

$$\hat{V}_n(t) = \hat{V}_{n-1}(t) + \frac{1}{2^n n! \sqrt{\pi}} H_{n-1}(t)Q_n(t). \tag{8.4}$$

For Laguerre polynomials

$$\int_0^\infty e^{-x} x^\alpha L_n^{(\alpha)}(x) L_m^{(\alpha)}(x) dx = \frac{\Gamma(n + \alpha + 1)}{n!} \delta_{m,n},$$

we define

$$V_n^\alpha(t) = - \int_0^\infty [L_n^{(\alpha)}(x)]^2 \log|x-t| x^\alpha e^{-x} dx.$$

Now we have

$$(L_n^{(\alpha)}(x))' = -L_{n-1}^{(\alpha+1)}(x), \quad (8.5)$$

and from Rodrigues' formula

$$e^{-x} x^\alpha L_n^{(\alpha)}(x) = \frac{1}{n} (e^{-x} x^{\alpha+1} L_{n-1}^{(\alpha+1)}(x))' \quad (8.6)$$

(see [15, pp. 101–102]). Integration by parts using (8.6) then gives

$$\begin{aligned} V_n^\alpha(t) &= -\frac{1}{n} \int_0^\infty L_n^{(\alpha)}(x) \log|x-t| d(e^{-x} x^{\alpha+1} L_{n-1}^{(\alpha+1)}(x)) \\ &= -\frac{1}{n} \int_0^\infty e^{-x} x^{\alpha+1} [L_{n-1}^{(\alpha+1)}(x)]^2 \log|x-t| dx \\ &\quad + \frac{1}{n} \int_0^\infty e^{-x} x^{\alpha+1} \frac{L_{n-1}^{(\alpha+1)}(x) L_n^{(\alpha)}(x)}{x-t} dx, \end{aligned}$$

where we used (8.5) in the first integral on the right. Now

$$\begin{aligned} \int_0^\infty e^{-x} x^{\alpha+1} \frac{L_{n-1}^{(\alpha+1)}(x) L_n^{(\alpha)}(x)}{x-t} dx &= \int_0^\infty e^{-x} x^{\alpha+1} L_{n-1}^{(\alpha+1)}(x) \frac{L_n^{(\alpha)}(x) - L_n^{(\alpha)}(t)}{x-t} dx \\ &\quad + L_n^{(\alpha)}(t) \int_0^\infty e^{-x} x^{\alpha+1} \frac{L_{n-1}^{(\alpha+1)}(x)}{x-t} dx, \end{aligned}$$

and since

$$\frac{L_n^{(\alpha)}(x) - L_n^{(\alpha)}(t)}{x-t} = -\frac{1}{n} L_{n-1}^{(\alpha+1)}(x) + P_{n-2}(x, t)$$

where P_{n-2} is a polynomial in x of degree at most $n-2$ with coefficients depending on t , we have by orthogonality

$$\int_0^\infty e^{-x} x^{\alpha+1} \frac{L_{n-1}^{(\alpha+1)}(x) L_n^{(\alpha)}(x)}{x-t} dx = -\frac{\Gamma(n + \alpha + 1)}{n!} - L_n^{(\alpha)}(t) Q_{n-1}^{(\alpha+1)}(t)$$

where

$$Q_{n-1}^{(\alpha+1)}(t) = \int_0^\infty e^{-x} x^{\alpha+1} \frac{L_{n-1}^{(\alpha+1)}(x)}{t-x} dx$$

is the Laguerre function of the second kind. This gives

$$nV_n^\alpha(t) = V_{n-1}^{\alpha+1}(t) - \frac{\Gamma(n + \alpha + 1)}{n!} - L_n^{(\alpha)}(t) Q_{n-1}^{(\alpha+1)}(t). \quad (8.7)$$

For the normalized weight function $w_\alpha(x) = x^\alpha e^{-x}/\Gamma(\alpha + 1)$, the orthonormal polynomials are $p_n(x) = (-1)^n \sqrt{n!}/(\alpha + 1)_n L_n^{(\alpha)}(x)$. Hence for the normalized potential, we have

$$\hat{V}_n^\alpha(t) := \frac{1}{\Gamma(\alpha + 1)} \int_0^\infty x^\alpha e^{-x} p_n^2(x) \log|x - t| dx = \frac{n!}{\Gamma(n + \alpha + 1)} V_n^\alpha(t)$$

hence the recurrence becomes

$$\hat{V}_n^\alpha(t) = \hat{V}_{n-1}^{\alpha+1}(t) - \frac{1}{n} - \frac{(n-1)!}{\Gamma(n + \alpha + 1)} L_n^{(\alpha)}(t) Q_{n-1}^{(\alpha+1)}(t). \quad (8.8)$$

9. Conclusion

In this paper, we have shown how the entropy of some classical orthogonal polynomials plays a role in some problems related to the harmonic oscillator and the Coulomb potential (hydrogen atom). We showed how this entropy for orthogonal polynomials is related to the distribution of zeros and to the mutual energy and logarithmic potential of some measures involving the zeros of the orthogonal polynomials. We analyzed the Gegenbauer polynomials, the Laguerre polynomials, and the Hermite polynomials in some detail. We obtained some closed formulas for the logarithmic energy of Chebyshev polynomials and showed how to obtain logarithmic potentials for measures $p_n^2(x) d\mu(x)$ recursively.

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References

1. J. C. Angulo and J. S. Dehesa, *Tight rigorous bounds to atomic information entropies*, J. Chem. Phys. **97** (1992), 6485–6495.
2. A. I. Aptekarev, V. S. Buyarov, and J. S. Dehesa, *Asymptotic behavior of the L^p -norms and the entropy for general orthogonal polynomials*, R. Akad. Nauk Mat. Sb. **185** (1994), 3–30 (In Russian); Russian Acad. Sci. Sb. Math. **82** (1995), 373–395.
3. A. I. Aptekarev, V. S. Buyarov, W. Van Assche, and J. S. Dehesa, *Asymptotics for entropy integrals of orthogonal polynomials*, Dokl. Russ. Acad. Sci. **346** (1996), 439–441.
4. A. I. Aptekarev, J. S. Dehesa, and R. J. Yáñez, *Spatial entropy of central potentials and strong asymptotics of orthogonal polynomials*, J. Math. Phys. **35** (1994), 4423–4428.
5. J. Avery, *Hyperspherical Harmonics: Applications in Quantum Theory*, Kluwer Academic, Dordrecht, (1988).
6. I. Białynicki-Birula and J. Mycielski, *Uncertainty relations for information entropy in wave mechanics* Commun. Math. Phys. **44** (1975), 129–132.
7. B. H. Bransden and C. J. Joachain, *Introduction to Quantum Mechanics*, Longmann, Essex, 1989.
8. L. S. Davtyan, G. S. Pogosyan, A. N. Sisakyan, and V. M. Ter-Antonyan, *On the hidden symmetry of a one-dimensional hydrogen atom*, J. Phys. A **20** (1987), 2765–2772.
9. H. Dette, *New identities for orthogonal polynomials on a compact interval*, J. Math. Anal. Appl. **179** (1993), 547–573.
10. I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series, and Products*, Academic Press, San Diego, 1980.
11. R. Loudon, *One-dimensional hydrogen atom*, Amer. J. Phys. **27** (1959), 649–655.
12. P. G. Nevai, *Orthogonal Polynomials*, Memoirs Amer. Math. Soc. **213**, Providence, RI, 1979.

13. M. M. Nieto, *Hydrogen atom and relativistic pi-mesic atom in N -space dimensions*, Amer. J. Phys. **47** (1979), 1067–1072.
14. E. M. Nikishin and V. N. Sorokin, *Rational Approximations and Orthogonality*, Translations of Mathematical Monographs **92**, Amer. Math. Soc., Providence, RI, 1991.
15. G. Szegő, *Orthogonal Polynomials*, Amer. Math. Soc. Colloq. Publ. **23**, Providence, RI, 1975.
16. W. Van Assche, *Asymptotics for orthogonal polynomials and three-term recurrences*, In: *Orthogonal Polynomials: Theory and Practice* (Ed. P. Nevai), NATO ASI series C **294**, Kluwer, Dordrecht, pp. 435–462.
17. ———, *Asymptotics for Orthogonal Polynomials*, Lecture Notes in Mathematics **265**, Springer-Verlag, Berlin, 1987.
18. W. Van Assche, R. J. Yáñez, and J. S. Dehesa, *Entropy of orthogonal polynomials with Freud weights and information entropies of the harmonic oscillator potential*, J. Math. Phys. **36** (1995), 4106–4118.
19. R. J. Yáñez, W. Van Assche, and J. S. Dehesa, *Position and momentum information entropies of the D -dimensional harmonic oscillator and hydrogen atom*, Phys. Rev. A **50** (1994), 3065–3079.

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