The Shannon, Rényi and Havrda-Charvat entropy functionals for the infinite well and quantum oscillator

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Abstract. We calculate the Shannon, Rényi and Havrda-Charvat entropy functionals ($\alpha = \beta = 1/2$) as functions of the excited states of the infinite potential well and quantum oscillator and show that all these entropy functionals represent the monotonous increasing functions of these states. From the mathematical point of view the presented entropy functionals are to be considered as equivalent uncertainty measures (spreads) of probability distributions. Though the Rényi and Havrda-Charvat entropy functionals represent equally well uncertainty measures as the Shannon entropy functional they are generally simpler evaluated mathematically than it.

1 Introduction

When teaching statistical physics, students are well-acquainted with the Gibbs-Shannon entropy. However, they are not generally acquainted with the fact that there exist a whole class of another measures of uncertainty apart of Shannon entropy. In physics, these measures of uncertainty, called in theory of probability as generalized entropies, become more and more important in quantum and statistical physics. Classical example is the Tsallis entropy [10] playing important role in statistical physics.

As is well-known, in theory of probability, there are basically two uncertainty measures of a random variable $\tilde{x}$, namely the moment and entropic ones (see, e.g. [4]). The *moment* uncertainty measures of $\tilde{x}$ contains in its definition components of its probability distribution *as well as* the corresponding values given on its probability states. A typical moment uncertainty measure of $\tilde{x}$ is its variance. The entropic uncertainty measure of a random variable contains *only* components of its probability distribution. The most important entropic measure of uncertainty of $\tilde{x}$ is the familiar Shannon *information* entropy [5]. If $\tilde{x}$ is a discrete random variable which takes the values $x_i\,,\, i = 1, 2, \ldots, n,$ with the probabilities $P(x_1), P(x_2), \ldots, P(x_n), \quad \sum_i P(x_i) = 1\,;\; P(x_i) \geq 0\,, i = 1, 2, \ldots, n,,$ then its information entropy is [5]

$$H(\tilde{x}) = -\sum_{i=1}^{n} P(x_i) \log P(x_i). \tag{1}$$

The Shannon information entropy for a discrete random variable with the finite probability states assumes a finite number. The transition from the discrete to the continuous Shannon information entropy is, however, not always unique and has still many open problems [1]. To a quantum continuous observable is assigned a continuous random variables $\tilde{x}_c$ with its probability density $p(x)$. Again, the typical moment measure of $\tilde{x}_c$ is its variance while its *entropic* uncertainty measure is its Shannon information entropy which is a function of its probability density $p(x)$ and consists of two terms

$$H(\tilde{x}_c) = S(p(x)) + S', \qquad S(p(x)) = -\int p(x) \log p(x)\; dx, \qquad S' = \lim_{\Delta x \to 0} \log \triangle x.$$

$H(\tilde{x}_c)$ with both terms S and S' *always* diverges, i.e. the information contain of $\tilde{x}_c$ is infinite. Usually, one "renormalizes" $H(\tilde{x}_c)$ by taking only the term $S(p(x))$ called the Shannon entropy functional (sometimes denoted as the differential entropy). $S(p(x))$ plays an important role in probability theory and statistics [6]. We refer to Karlin and Rinott [7] for applications of $S(p(x))$ in probability theory and statistics.

From the mathematical point of view, $S(p(x))$ can be taken as a formula for expressing the spread of any normed single-valued function (the probability density belongs to this class of functions). The Shannon entropy functional was studied just at the beginning of information theory [8]. Since that time, besides $S(p(x))$, several other similar entropy functionals were introduced and studied in information theory. The majority of them depend on certain parameters. As such, they form a whole family of different entropy functionals (including $S(p(x))$ as a special case). In a sense, they are generalization of $S(p(x))$ and express likewise the uncertainty measure (spread) of $p(x)$. Two most familiar are

(i) The Rényi entropy functional $S_\alpha^{(R)}$ given as [8]

$$S_\alpha^{(R)}(p(x)) = \frac{1}{1-\alpha}\log\left[\int_{-\infty}^{\infty}[p(x)]^\alpha dx\right] \qquad \alpha \in R. \tag{a}$$

(ii) The Havrda-Charvat entropy functional $S_\beta^{(HC)}$ given as [9]

$$S_\beta^{(HC)}(p(x)) = \frac{1}{1-\beta}\left[\int_{-\infty}^{\infty}[p(x)]^\beta dx - 1\right] \qquad \beta \in R. \tag{b}$$

A quick look shows that $S_\alpha^{(R)}$ and $S_\beta^{(HC)}$ are functionally related. Note that $S_\alpha^{(R)}, S_\beta^{(HC)}$ tend to $S(p(x))$ as α, β tends to 1. In some instances, it is simpler to compute $S_\alpha^{(R)}, S_\beta^{(HC)}$ and then recover $S(p(x))$ by taking limits $\alpha, \beta \to 1$.

According to experimental arrangement a particle can be described by different wave functions $\phi(z)$ and so with different position or momentum probability density functions $p(z) = |\phi(z)|^2$. When taking the Rényi and Havrda-Charvat entropy functionals with $\alpha = \beta = 1/2$ as the uncertainty measures of $p(z)$, then the *integrand* in (a) and (b) becomes simply $p(z)^{1/2} = |\phi(z)|$. This is why we focus our attention on these entropy functionals which we denote as RF and HCF

$$RF(p(z)) = 2\log\left[\int_{-\infty}^{\infty} p(z)^{1/2}dx\right]$$

and

$$HCF(p(z)) = 2\left[\int_{-\infty}^{\infty} p(z)^{1/2}dz - 1\right],$$

respectively. For the position probability density $p(x) = |\varphi(x)|^2$ the Shannon, Rényi and Havrda-Charvat entropy functionals become

$$S(\varphi(x)) = \int_{-\infty}^{\infty} |\varphi(x)|^2 \log |\varphi(x)|^2 dx,$$

$$RF(\varphi(x)) = 2\log\left[\int_{-\infty}^{\infty} |\varphi(x)| dx\right] \qquad (a')$$

and

$$HCF(\varphi(x)) = 2\left[\int_{-\infty}^{\infty} |\varphi(x)| dx - 1\right], \qquad (b')$$

respectively. We see that the integrand in (a') and (b') represents the absolute value of the position wave function.

In Sections 2 and 3 we calculate the position and momentum Rényi and Havrda-charvat functionals, RF and HCF, for the excited states ($n \in [1, 40]$) of the infinite well and quantum oscillator and compare them with the corresponding Shannon entropy functional. In Section 4 we summarize the most important results.

2 The Shannon, Rényi and Havrda-Charvat entropy functionals for the infinite well

As is well-known, the infinite potential well is a quantum system defined as ($\hbar = 1$) [2]

$$U(x) = \begin{cases} 0 & \text{for} \quad |x| \le a \\ +\infty & \text{for} \quad |x| > a \, , \end{cases} \qquad (2)$$

where $U(x)$ is the potential. Its position and momentum wave functions are

$$\psi_n(x) = \begin{cases} \frac{1}{\sqrt{a}} \sin\left[\frac{\pi n}{2a}(x-a)\right] & \text{for} \quad |x| \le a \\ 0 & \text{for} \quad |x| > a \end{cases}, \qquad (3)$$

$$\phi_n(p) = \sqrt{\frac{\pi n^2}{2a^3}} \frac{\sin(ap - \frac{\pi}{2} n)}{\left(p^2 - \frac{\pi^2 n^2}{4a^2}\right)}, \qquad (4)$$

respectively.

Inserting the position probability density, $p(x) = |\psi_n(x,a)|^2$ into $S(p(x))$, $RF(p(x))$ and $HCF(p(x))$ we get [3]

$$S(\psi_n(x,a)) = -\int_{-a}^{a} |\psi_n(x,a)|^2 \log |\psi_n(x,a)|^2 dx = \ln(4a) - 1. \tag{5}$$

With

$$\Psi(a) = \int_{-a}^{a} \psi_n(x,a)dx = \int_{-a}^{a} \left| \frac{1}{\sqrt{a}} \sin\left(\frac{n\pi(x-a)}{2a}\right) \right| dx = \frac{4\sqrt{a}}{\pi}$$

we have

$$RF(\psi_n(x,a)) = 2\log\Psi(a) = 2\log\left[\frac{4\sqrt{a}}{\pi}\right] \tag{6}$$

$$HCF(\psi(x,a)) = 2\left[\Psi(a) - 1\right] = 2\left(\frac{4\sqrt{a}}{\pi} - 1\right).$$

We see that all the considered entropy functionals for the infinite well are independent of n.

Inserting the momentum probability density into above functionals we obtain

$$S(\phi_n(p)) = -\int_{-\infty}^{\infty} |\phi_n(p)|^2 \log |\phi_n(p)|^2 dp.$$

With

$$\Phi_W(n,a) = \int_{-\infty}^{\infty} |\phi_n(p,a)| dp$$

we have

$$RF(\phi_n(p)) = 2\left[\log\left(\Phi_W(n,a)\right)\right]$$

and

$$HCF(\phi_n(p)) = 2\left[\Phi_W(n,a) - 1\right].$$

$\Phi_W(a,n)$ represents the integral of the square of the momentum density function of the infinite well. The corresponding indefinite integral can be evaluated analytically (using the software MATHEMATICA 5) for an arbitrary a and n yielding

$$\Phi_W(a,n) = \int |\phi_n(p,a)| dp = \frac{1}{8n\sqrt{\pi}} \{n\sqrt{a} x^{(+)} x^{(-)} \cos(ap - \frac{n\pi}{2})$$

$$+\sin(ap-\frac{n\pi}{2})(x^{(+)}x^{(-)})^{-1}IC(x^{(-)})\sin(y^{(-)})-IC(x^{(+)})\sin(y^{(+)})$$
$$-\cos(y^{(-)})IS(x^{(-)})+\cos(y^{(+)})IS(x^{(+)})\},$$

where $x^{(+)}=a(p+n\pi)$, $x^{(-)}=a(p-n\pi)$, $y^{(+)}=(1+2a)n\pi/2$ and $y^{(-)}=(1-2a)n\pi/2$. IS and IC denote the integralsine and integralcosine, respectively.

The dependence of $\Phi_W(n,a)$ $(a=1)$ versus n is depicted in Fig.1. From Fig.1 it follows that

$$\Phi_W(n,a)<\Phi_W(n+1,a),$$

i.e. the spread of position wave function increase with increasing n.

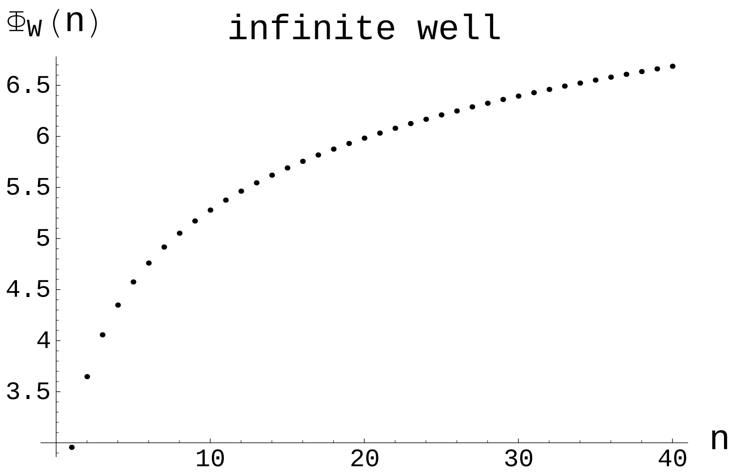

Figure 1: $\Phi_W(n)$ for momentum of the infinite well $(a=1)$ as a function of n.

The dependence of the Shannon, Rényi and Havrda-Charvat entropy functionals for momentum wave function on n are depicted in Fig.2. We see that the momentum Shannon entropy functional for the infinite well, as a function of n, is always smaller than the corresponding RF and HCF. All these entropy functionals exhibit a correlated increase with n, which corresponds to the increase of uncertainties of the momentum probability density.

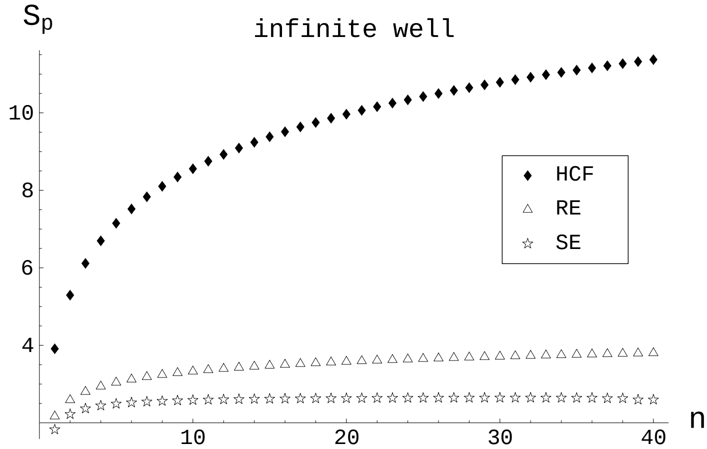

Figure 2: $S^{(HC)}_{1/2}(\psi_n(p)) - HCF$, $S^{(R)}_{1/2}(\psi_n(p)) - RE$ and Shannon entropy functional $S(\psi_n(p)) - SE$ for momentum of well (a=1) as a function of n.

3 The Shannon, Rényi and Havrda-Charvat entropy functionals for a quantum oscillator

The wave function of a quantum harmonic oscillator reads as

$$\varphi_n(x) = C_n H_n(x) \exp{(-x^2/2)},$$

where $C_n = (n!2^n\sqrt{\pi})^{-1/2}$ is the norm constant and $H_n(x)$ is Hermite polynomial of n-th degree [2]. Since the wave function in momentum representation is the Fourier transform of position wave function, having similar form as position one, we will investigate only the position probability density assigned to a quantum state of quantum oscillator. The Shannon entropy functional of position probability density of quantum oscillator is given as

$$S(\varphi_n(x)) = -\int_{-\infty}^{\infty} |\varphi_n(x)|^2 \log|\varphi_n(x)|^2 dx.$$

With

$$\Phi_{QO}(n) = \int_{-\infty}^{\infty} |\varphi_n(x)| dx$$

we get

$$RF(n) = 2\left[\log\left(\Phi_{QO}(n)\right]\right. \quad \text{and} \quad HCF(n) = 2\left[\Phi_{QO}(n) - 1\right]$$

The position $S(\varphi_n(x))$,$RF(\varphi_n(x))$ and $HCF(\varphi_n(x))$ as functions of n, we have calculated numerically. The dependence of $\Phi_{QO}(n)$ is depicted in Fig.3. The position Shannon entropy functional of the excited states of quantum oscillator as a function of n has been also calculated in [13] and [12]. As seen in Fig.4, the Shannon entropy functional, HCF and RF for the excited states of quantum oscillator show correlated enlargement with n however, with the different increase.

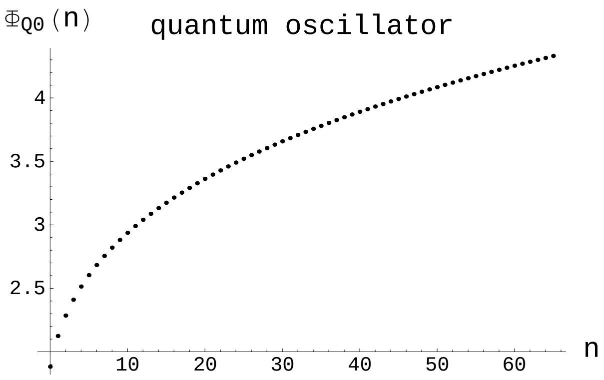

Figure 3: $\Phi_{QO}(n)$ as a function of n (a=1).

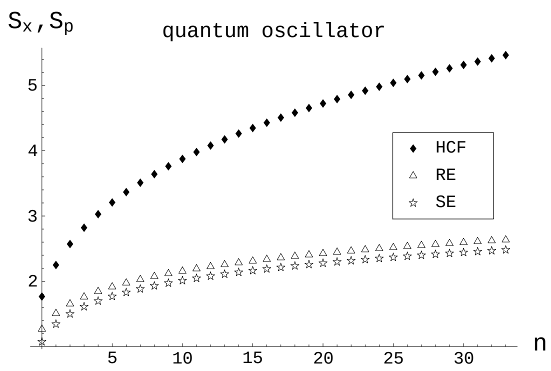

Figure 4: $S^{(HF)}_{1/2}(\varphi_n(x)) - HCF$, $S^{(R)}_{1/2)}(\varphi_n(x)) - RE$ and Shannon entropy functional $(S(\varphi_n(x)) - SE)$ for position of the quantum oscillator as a function of n (a=1).

4 Conclusions

(i) Figs. 1 and 3 show that $\Phi_W(n)$ and $\Psi_{QO}(n)$ represent sequences of n which monotonously increase with the excited states of the infinite well as well as quantum oscillator. This means that spreads of the probability distributions assigned to corresponding wave functions enlarge as the energy eigenvalues increases.

(ii) As seen in Fig. 2 all entropy functionals exhibit correlated sequences of n however, with different degree of increase.

(iii) Striking feature of graphs depicted in Fig.2 and 4 is a small difference between the values of $S(n)$ and $RF(n)$.

(v) All the considered entropy functionals belong to the set of uncertainty measures of probability distribution in that all of them enlarge as their uncertainty enlarge. $HCF(p(x))$ and $HCF(p(x))$ equally well express the spreads of the probability density functions as $S(p(x))$.

(vi) In the literature the entropic uncertainty relation is often defined as the sum of position and momentum of information entropies of two continuous non-commuting observables . This is strictly speaking incorrect because the information entropy of any continuous probability simply diverges. The Shannon entropy functional resembles only in the form the Shannon information entropy but in fact it does not express the information content of the continuous probability distribution but it is only one element of the class of general uncertainty measures.

(v)From the purely mathematical point of view, $S(p(x))$, $S^R(p(x))$ and $S^{HC}(p(x))$ have to be taken as different formulas for expressing the spread of any normed single-valued function (the probability density belongs to this class of functions). Generally, $S(p(x))$, $S^R(p(x))$ and $S^{HC}(p(x)$ assign to a probability density function (which belongs to the class of functions $L^2(R^1)$) a real number S through a mapping $L^2(R_1) \to S$. S is a monotonously increasing function of the degree of spread of $p(x)$.

(vi) As it is well-known, the Shannon entropy functionals of some continuous observables contain complicated integrals which often are difficult to compute analytically and even numerically. Everybody who tried to calculate analytically the Shannon entropy functionals of the continuous observables, became aware of how difficult this may be [13]. On the other side, the Rényi and Havrda-Charvat entropy functionals for a number of quantum systems are generally easier to handle mathematically than the Shannon one.

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