acta physica slovaca vol. 46 No. 5, 615 – 621 October 1996

ZERO-CONTINGENT ENTROPY OF QUANTUM STATES OF A HYDROGEN ATOM

R. Charvot, V. Majerník
Department of Theoretical Physics
Palacký University Svobody 26 771 46 Olomouc, Czech republic

Received 9 July 1996 , accepted 5 September 1996

We calculated the zero-contingent entropy for the position of electron in H-atom as a function of its quantum numbers and compared it with the corresponding value of the Shannon entropy. The values of zero-contingent entropy of quantum states of H-atom correlate well with the corresponding values of Shannon's entropy. This points out that, besides the Shannon entropy, the zero-contingent entropy represents an appropriate, and mathematically rather simple, measure of the spreading out of the wave functions in H-atom.

1. Introduction

There has been a considerable recent interest in determining various measures for uncertainty of the observables (e.g. dispersion, entropy, etc.) for certain quantum systems in order to find different types of the uncertainty relations [1,2,3]. In accordance with the present understanding the quantum system is described by a complex function $\psi(x,t)$ which is linked with the function of finding a particle at position x and time t by the equation $P(x,t) = |\psi(x,t)|^2$. As is well-known to any quantum observable a random variable can be ascribed which is generally given by the probabilistic scheme

S	S_1	S_2	...	S_n
P	$\|\psi_1(x,t)\|^2$	$\|\psi_2(x,t)\|^2$	...	$\|\psi_n(x,t)\|^2$
x	x_1	x_2	...	x_n

In the first, second and third row in this scheme there are quantum states, their probabilities and the corresponding eigenvalues, respectively. In the theory of probability there are essentially two types of measures of the uncertainty of a random variable [4].

- the *moment* measures of uncertainty of random variables given by means of the scatter of its values determined generally by its central statistical moments
- the *probabilistic* or *entropic* measures of uncertainty containing in their expressions only elements of the probability distribution of a random variable and determining the sharpness of its probability distribution.

0323-0465/96

If $\tilde{x}$ is a discrete random variable given by probabilistic scheme

S	S_1	S_2	...	S_n
P	$P(x_1)$	$P(x_2)$	...	$P(x_n)$
x	x_1	x_2	...	x_n

then its $k-th$ statistical moment is

$$m^{(k)} = \sum_{i=1}^{n}(x_i - m_o)^k P(x_i),$$

where

$$m_0 = \sum_{i=1}^{n} x_i P(x_i)$$

If $\tilde{x}_c$ is a continuous random variable with the probability density function $p(x)$, then its k-th central statistical moment is

$$m^{(k)} = \int_{\infty}^{\infty}(x - x_0)^k p(x)dx,$$

where

$$x_0 = \int_{-\infty}^{\infty} x p(x)dx.$$

Especially, the dispersion, representing the second central moment

$$\sigma = \int_{-\infty}^{\infty}(x - x_0)^2 p(x)dx,$$

is often used as a measure for the accuracy of a measurement. The moment measures of uncertainty also entered in the standard formulation of Heisenberg-type uncertainty relations in quantum physics [5].
The most important entropic measures of uncertainty of a random variable, characterized by the probability distribution function $P(x)$, is given by the general integral [6]

$$H = -\int P(x)\log P(dx)$$

and is called Shannon entropy. If $\tilde{x}$ is a discrete random variable which takes the values x_i, $i = 1,2,\ldots,n$, with the probabilities $\mathbf{P} = \{P(x_1), P(x_2), \ldots, P(x_n)\}$, $\sum P(x_i) = 1$; $P(x_i) \geq 0$, $i = 1,2,\ldots,n,$, then its Shannon entropy is given by the formula

$$H(\mathbf{P}) = H(x) = -\sum P_i \log P_i \tag{1}$$

The entropy of the continuous random variable $\tilde{x}$, characterized by the function of the probability density $p(x)$ has the form

$$H(\tilde{x}_c) = H^{(1)} + H^{(2)} \tag{2}$$

where $H^{(1)}$ is the so-called differential entropy

$$H^{(1)} = -\int p(x)\log p(x)\ dx \tag{3}$$

and $H^{(2)}$ represents the diverging term

$$H^{(2)} = \lim_{x\to 0}\log \Delta x\quad . \tag{4}$$

It is interesting that besides the Shannon entropy there exists a set of non-standard entropies which serve as certain entropic measures of uncertainty of random variables as well (for a review see [12]). We mention only the most important of them [7]

- The β-entropy

$$H_\beta = \sum_{i=1}^{n} P(x_i)[1 - P(x_i)^\beta]^{1/\beta} + \sum_{i=1}^{n} P(x_i)[1 - P(x_i)],$$

where β is a parameter, $\beta \in \langle 0,1)$.

- The contingent entropy

$$H_\alpha = \sum_{i=1}^{n} P(x_i)^{1-\alpha}[1 - P(x_i)]^\alpha + \sum_{i=1}^{n} P(x_i)[1 - P(x_i)]$$

where $\alpha \in \langle 1,2\rangle$ is a parameter.
In the limiting case, if $\beta \to 0$, β-entropy, H_β, gets the form

$$H_0(\tilde{x}) = H_\beta(\tilde{x}) = \sum_{i=1}^{n} P(x_i)[1 - P(x_i)] \tag{a}$$

and is called the zero-contingent entropy.
All these measures have similar properties as the Shannon entropy but they are generally more simple to handle mathematically (they have no logarithm in their definitions). The aim of this article is to show that one of these non-standard entropic measures, the zero-contingent entropy, can be used as a possible measure of uncertainty of a quantum observable. The integrals determining this entropy can be in principle calculated analytically though by a lengthy procedure. This is not generally the case for the Shannon entropy. In what follows we calculate the zero-contingent entropy for the position of electron which occurs in various quantum states in H-atom. The values of this entropy correlate with the values of the Shannon entropy for the corresponding quantum states of H-atom. Therefore, the zero-contingent entropy represents an alternative measure for uncertainty of a quantum observable.

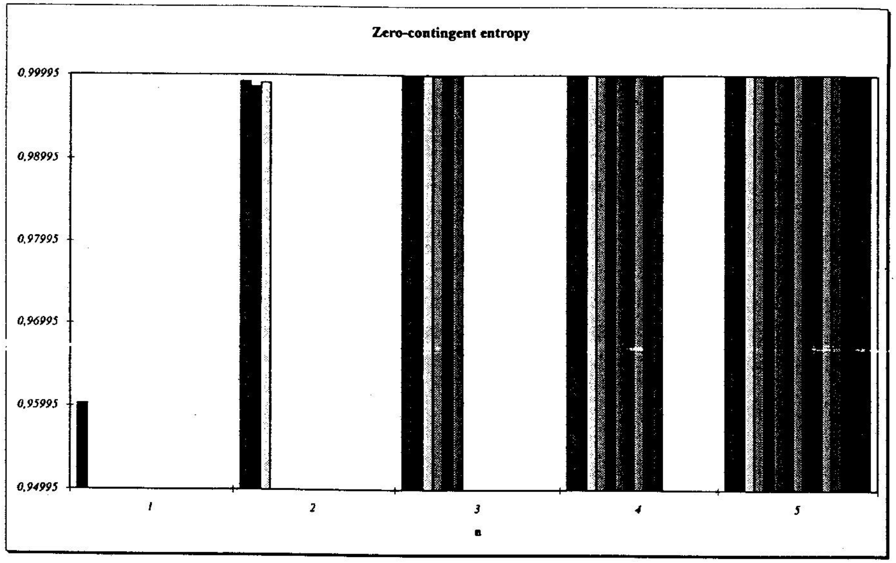

Fig. 1. Zero-contingent entropies of quantum states of H-aton (broad scale)

2. Zero-contingent entropy for position in H-atom

The simplest quantal system of two bodies with the Coulomb interaction represents the hydrogen atom. If E is energy of the electron-proton system then the wave function $\psi(r,\vartheta,\varphi)$ of electron is a solution of the Schrödinger equation [8]

$$\left[-\frac{\hbar^2}{2m}\,\Delta-\frac{e^2}{r}\right]\psi(r,\vartheta,\varphi)=E\psi(r,\vartheta,\varphi) \quad . \tag{5}$$

Carrying out the separation of angular and radial variables the eigensolutions of (5) for eigenenergies E_n are

$$\psi_{n,l,\lambda}(r,\vartheta,\varphi)=\chi_{n,l}Y^l_\lambda(\vartheta,\varphi) \quad ,$$

where $\chi_{n,l}$ are radial functions and Y_λ are the spherical harmonics. n, l and λ is radial (principal), azimuthal and magnetic quantum number, respectively. The probability of finding electron within the volume element, $d\tau$, is $dP=\psi\psi^* d\tau$ and the corresponding probability density

$$p(r,\vartheta,\varphi)=\frac{dP}{d\tau}=\psi\psi^*=|\psi_{nl\lambda}(r,\vartheta,\varphi)|^2 \quad .$$

The distribution $p(r,\vartheta,\varphi)$ can be experimentally determined with the aid of electron scattering experiments [13]. By means of these experiments one can find the cross section and the rates of collisional ionization of H-atom in its different quantum states.The spreading of wave function of H-atom, whose measure is the zero-contingent entropy, is functionally linked with the above-mentioned measurable quantities.

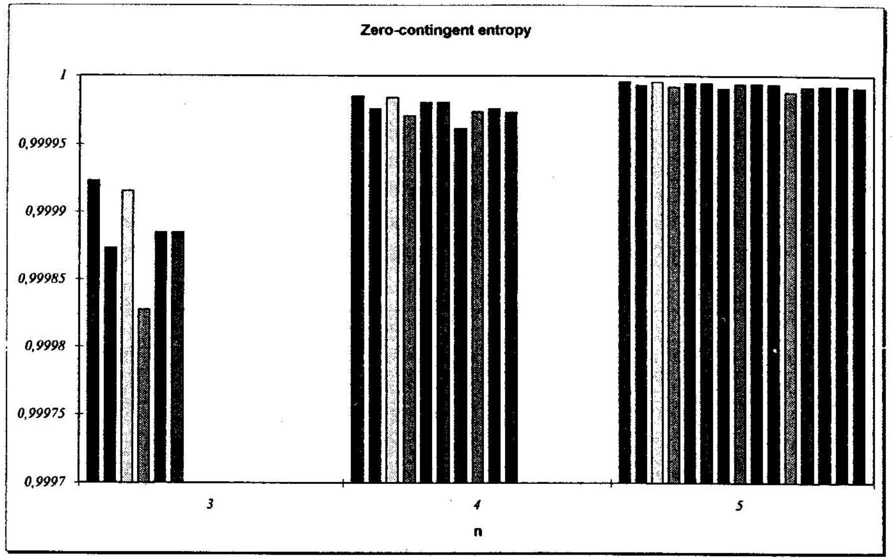

Fig. 2. Zero-contingent entropies of quantum states of H-atom (fine scale).

The zero-contingent entropy for the continuous random variable $\tilde{x}$ with the density probability function, $p(x)$, turns out to be

$$H_0(\tilde{x}_c)=S=\int_{-\infty}^{\infty}p(x)[1-p(x)]dx=1-\int_{-\infty}^{\infty}(p(x))^2dx. \tag{b}$$

We next calculate the zero-contingent entropy for the quantum states of hydrogen atom in that we insert the corresponding probability density function of electron in H-atom in the formula for zero-contingent (Eq.(b))

$$S_{nl\lambda}=1-\int_0^\infty\int_0^{2\pi}\int_0^{2\pi}|\phi_{nl\lambda}(r,\vartheta,\varphi)|^4d\tau(r,\vartheta,\varphi)$$

The zero-contingent entropy, $S_{nl\lambda}$, gives the uncertainty of the position of electron in H-atom and its magnitude represents also a measure of spreading out of the considered wave function in H-atom. We have calculated the zero-contingent position entropies of H-atom as a function of its quantum numbers (The calculation were performed using *Mathematica* [11]). The numerical values of the zero-contingent entropy of H-atom are given in Table 1 and graphically represented in Fig.1 and 2. We see that the $S_{nl\lambda}$ represents a monotonically increasing function of principal number n having minimal value for $n=1$. This corresponds with the behaviour of other measures for uncertainty especially that of the Shannon entropies [9,10]. For fixed n and different l and λ we found also correlated values of zero-contingent entropy with the Shannon entropies presented in [10]. The great disadvantage of the zero-contingent entropy is that it gets-values rather close to 1 which causes that the individual values differ only little from each other and, therefore, the correspondent integrals must be calculated with high accuracy.

The comparison of the zero-contingent entropies and Shannon's entropies for H-atom shows that the Shannon's entropies are much more dispersed than the zero-contingent entropies. The larger sensitivity of Shannon's entropy on the share of wave function can be explained by the occurrence of logarithm in its definition which is much more sensitive for the share of the wave function than power function occurring in the zero-contingent entropy.

n	l	λ	$S_{nl\lambda}$	n	l	λ	$S_{nl\lambda}$	n	l	λ	$S_{nl\lambda}$
1	0	0	0.96021126	4	1	1	0.99998411	5	2	1	0.99999486
2	0	0	0.99922288	4	2	0	0.99997097	5	2	2	0.99999486
2	1	0	0.99860118	4	2	1	0.99998065	5	3	0	0.99999095
2	1	1	0.99906745	4	2	2	0.99998065	5	3	1	0.99999384
3	0	0	0.99992325	4	3	0	0.99996159	5	3	2	0.99999437
3	1	0	0.99987336	4	3	1	0.99997386	5	3	3	0.99999374
3	1	1	0.99991557	4	3	2	0.99997609	5	4	0	0.99998811
3	2	0	0.99982731	4	3	3	0.99997344	5	4	1	0.99999176
3	2	1	0.99988487	5	0	0	0.99999590	5	4	2	0.99999263
3	2	2	0.99988487	5	1	0	0.99999343	5	4	3	0.99999266
4	0	0	0.99998524	5	1	1	0.99999562	5	4	4	0.99999143
4	1	0	0.99997616	5	2	0	0.99999229				

3. Conclusion

From what has been said so far it follows that
(i) The uncertainty in the electron position in H-atom can be determined by different entropic measures. Among these entropic measures the zero-contingent entropy seems especially suitable for the calculation of this position uncertainty.
(ii) The values of zero-contingent entropy for localization of electron of quantum states in H-atom correlate with the corresponding values of the Shannon entropies.
(iii) There is a disadvantage for the use of zero-contingent entropy in that it yields very small differences between the different quantum states.
Summing up we can conclude that the zero-contingent entropy can be considered as an alternative entropic measure of uncertainty besides the Shannon entropy.

References

[1] I. Bialycki-Birula, J. Mycielski: *Commun. Math. Phys.* **44** (1975) 129
[2] D. Deutsch: *Phys. Rev. Lett.* **50** (1983) 631
[3] V. Majernik, T. Opatrny: *J. Phys. A: Math. Gen.* **29** (1996) 2187
[4] W. Feller: *An Introduction to Probability Theory and its Applications.* Vol. I. (Wiley,New York 1968).

[5] J.B.M. Uffink, J. Hilgevoord: *Found. Phys.* **15** (1985) 925
[6] A.N. Kolmogoroff: *Theorie der Nachrichtungsubertragung* (D.Verlag d. Wiss.,Berlin, 1957)
[7] V. Majernik, B. Mamojka: *Phys. Scr.* **44** (1991) 412
[8] E. Merzbacher: *Quantum Mechanics* 7th edn (New Your : Wiley, 1967)
[9] V. Majernik: *Acta Phys. Slovaca* **25** (1995) 75
[10] R.J. Yanes, W. van Assche, J.D. Dehese: *Phys. Rev.* **A50** (1994) 3065
[11] S. Wolfram: *Mathematica, a System for Doing Mathematics by Computer* (Redwood City: Addison-Wesley, 1991)
[12] J. Vajda: *Information theory and statistical decisions* (in Czech, Bratislava: Alfa, 1982)
[13] L. Vriens, A.H.M. Smeets: *Phys. Rev.* **A22** (1980) 940