Lower Bound for LMC complexity measure

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(Dated: April 24, 2009)

Abstract

Lower bound for the shape complexity measure of López-Ruiz-Mancini-Calbet (LMC), $C_{LMC}$, is derived. Analytical relations for simple examples of the harmonic oscillator, the hydrogen atom and two-electron ‘entangled artificial’ atom proposed by Moshinsky are derived. Several numerical examples of the spherically confined model systems are presented as the test cases. For the homogeneous potential, $C_{LMC}$ is found to be independent of the parameters in the potential which is not the case for the non-homogeneous potentials.
I. INTRODUCTION

There are several statistical measures of complexity [1, 2]. A given measure becomes significant when a rigorous bound on it is known to exist. In this letter, we focus on the LMC (López-Ruiz-Mancini-Calbet) complexity [1], $C_{LMC}$, with the aim of deriving a general lower bound for it. The lower bound is tested by presenting (a) the analytical expressions for some simple systems: the harmonic oscillator, the hydrogen atom and two-electron atom proposed by Moshinsky [3] and (b) the numerical calculations on the spherically confined model one and two electron systems [4, 5, 6, 7].

Consider a $D$-dimensional distribution function $f(r)$, with $f(r)$ nonnegative and $\int f(r) dr = 1$; $r$ stands for $r_1, ..., r_D$. The Shannon entropy [8] and the Shannon entropy power are defined as

$$S_f = - \int f(r) \ln f(r) dr,$$

$$H_f = e^{S_f},$$

respectively. The so-called disequilibrium $D$ has the form

$$D_f = \int f^2(r) dr.$$

The definition of the LMC complexity measure is [9]

$$C_{LMC} = H.D$$

It is known [9] that the complexity corresponding to probability distributions given by rectangular, triangular, Gaussian and exponential functions in one-dimensional position space is given by $1$, $(2/3)(e^{1/2})$, $(e^{1/2})/2$, and $e/2$, respectively. The rectangular probability distribution, by definition, corresponds to the minimum statistical complexity. We shall now derive the lower bound for $C_{LMC}$ corresponding to a given one-electron density.

II. INEQUALITY FOR THE LMC COMPLEXITY

To derive a lower bound for the LMC complexity we cite Theorem 2 of the paper of Yáñez, Angulo and Dehesa [10]. The position-space entropy $\tilde{S}_e$ of an $N$-electron system in
a physical state characterized by the (normalized to $N$) one-electron density $\rho(\mathbf{r})$ fulfills the inequality
\[
\tilde{S}_o + \ln g(\mathbf{r}) \leq N \ln \left( \frac{\int \rho(\mathbf{r}) d\mathbf{r}}{N} \right),
\]
where $g(\mathbf{r})$ is an arbitrary positive function. From the relationship between the Shannon entropies coming from densities normalized to 1 and $N$ [10]:
\[
S_f = \frac{\tilde{S}_o}{N} + \ln N
\]
and taking $g = f^2$, we obtain the inequality
\[
S_f + \ln \left( \int f^2(\mathbf{r}) d\mathbf{r} \right) \geq 0
\]
From the definition of the LMC complexity (4) we obtain the upper bound
\[
\ln C_{LMC} \geq 0
\]
or
\[
C_{LMC} \geq 1.
\]
In the next section analytical expressions are presented for some simple systems, such as the harmonic oscillator, the hydrogen atom and two-electron atom proposed by Moshinsky.

III. ANALYTICAL EXAMPLES

Consider first the one dimensional box problem i.e. the infinite square well in one dimension: $V(x) = 0$, if $|x| < a$ and $V(x) = \infty$, if $|x| > a$. Even solutions are
\[
\psi_{e,n} = A \cos \left( \frac{n \pi x}{2a} \right),
\]
if $|x| < a$. Odd solutions are
\[
\psi_{o,n} = B \sin \left( \frac{n \pi x}{2a} \right),
\]
if $|x| < a$. $n = 1, 2, ..., A = B = 1/a^{1/2}$ is the normalization constant. The disequilibrium takes the form:

$$D = \frac{3}{4a}$$  \hspace{1cm} (12)

for all eigenfunctions. The Shannon entropy can be written as

$$S_e = \ln a - 1 - \int_{-1}^{1} \ln \left( \cos \left( \frac{n\pi u}{2} \right) du \right),$$  \hspace{1cm} (13)

for the even solutions and

$$S_o = \ln a - 1 - \int_{-1}^{1} \ln \left( \sin \left( \frac{n\pi u}{2} \right) du \right),$$  \hspace{1cm} (14)

for the odd solutions. Eqs. (12), (13) and (14) lead to the expression

$$\ln C_{LMC} = S + \ln D = \ln \left( \frac{3}{4} \right) - 1 - \int_{-1}^{1} \ln \left( \cos \left( \frac{n\pi u}{2} \right) du \right)$$  \hspace{1cm} (15)

and

$$\ln C_{LMC} = S + \ln D = \ln \left( \frac{3}{4} \right) - 1 - \int_{-1}^{1} \ln \left( \sin \left( \frac{n\pi u}{2} \right) du \right)$$  \hspace{1cm} (16)

for the even and odd cases, respectively. So the complexity for a particle in a one-dimensional box contains, except the quantum number $n$, no parameter not only in the ground- but excited states, as well. It is possible to extend this result for the particle in a spherical box, PIASB, represented by the radial Schrödinger equation

$$\frac{d^2 R_{nl}}{dr^2} + \frac{2}{r} \frac{d R_{nl}}{dr} + \left[ 2E - \frac{l(l+1)}{r^2} \right] R_{nl} = 0$$  \hspace{1cm} (17)

where the radial wave function $R_{nl}(r)$ is given by

$$R_{nl} = N j_l(r\sqrt{2E})$$  \hspace{1cm} (18)

where $j_l$ is the Bessel function of the first kind of order $l$ and $N$ denotes the normalization constant. With the Dirichlet boundary condition imposed according to $R_{nl}(r_c) = 0$, one obtains through the condition $j_l(r_c\sqrt{2E}) = 0$ or $(r_c\sqrt{2E}) = u_{l,k}$, the energy levels given by

$$E_{k,l} = \frac{u_{l,k}^2}{2r_c^2},$$

where $u_{k,l}$ denotes the $k^{th}$ zero of $j_l$. For the ground state, one obtains for the
The disequilibrium

\[ D = \frac{Si(2\pi) - \frac{Si(4\pi)}{2}}{(r_c)^3} = \frac{0.6720709}{(r_c)^3}, \]  

\[ (19) \]

The Shannon entropy can be written as

\[ S_r = \ln(8\pi r_c^3) - 3 + \frac{Si(2\pi)}{\pi} \]  

\[ (20) \]

From Eqs. (19) and (20) we obtain the relation

\[ C_LMC = 1.3207394, \]  

\[ (21) \]

which is constant with respect to the radius of confinement \( r_c \). A similar analysis in the momentum space using the Fourier transform of the position space wave function in the case of PIASB leads to \( C_LMC = 1.517215 \). As our second example, we consider free linear harmonic oscillator with potential \( V = \frac{1}{2}kx^2 \). Then the ground-state density has the form

\[ \rho = \frac{k^{1/4}}{\pi^{1/2}} \exp\left(-\frac{k^{1/2}}{2}x^2\right). \]  

\[ (22) \]

We can immediately obtain the Shannon entropy:

\[ S = -\ln\left(\frac{k^{1/4}}{\pi^{1/2}}\right) + \frac{1}{2} \]  

\[ (23) \]

and the disequilibrium:

\[ D = \frac{k^{1/4}}{(2\pi)^{1/2}}. \]  

\[ (24) \]

From Eqs. (23) and (24) we are led to the relation

\[ \ln C_LMC = S + \ln D = \frac{1}{2}(1 - \ln 2). \]  

\[ (25) \]

Thus the complexity of the linear harmonic oscillator in the ground state is

\[ C_LMC = e^{\frac{1}{2}(1-\ln 2)}. \]  

\[ (26) \]

This is a remarkable result as it is a constant, independent of \( k \).
The third example is the free hydrogen atom, or hydrogen-like atomic ions. The ground-state density takes the form
\[
\rho = \frac{Z^3}{\pi} \exp(-2Zr), \quad (27)
\]
where \(Z\) is the atomic number. The Shannon entropy can be written as
\[
S = 3 - \ln \left( \frac{Z^3}{\pi} \right), \quad (28)
\]
while the disequilibrium takes the form:
\[
D = \frac{Z^3}{8\pi}. \quad (29)
\]
Eqs. (28) and (29) lead to the expression
\[
\ln C_{LMC} = S + \ln D = 3(1 - \ln 2), \quad (30)
\]
so the complexity of hydrogen-like atomic ions in the ground state is
\[
C_{LMC} = e^{3(1-\ln 2)}. \quad (31)
\]
Here, again there is no parameter in the result.

In the Moshinsky model two electrons with antiparallel spins interact harmonically in isotropic harmonic confinement. The Hamiltonian has the form
\[
H = \frac{1}{2} \left( -\nabla_1^2 + r_1^2 \right) + \frac{1}{2} \left( -\nabla_2^2 + r_2^2 \right) + \frac{1}{2}Kr_{12}^2, \quad (32)
\]
where
\[
r_{12} = r_1 - r_2 \quad (33)
\]
and \(K\) is the coupling constant. Introducing relative (Eq.(33)) and centre of mass coordinates
\[
R = \frac{1}{2} (r_1 + r_2) \quad (34)
\]
the Schrödinger equation can be separated leading to the equations

\[ \left( -\frac{1}{2} \nabla^2_R + 2 R^2 \right) \Psi^{CM} = E^{CM} \Psi^{CM} \]  

(35)

and

\[ \frac{1}{2} \left( -\nabla^2_{r_{12}} + \frac{1}{2} \left( \frac{1}{2} + K \right) r_{12}^2 \right) \Psi^{RM} = E^{RM} \Psi^{RM}. \]  

(36)

The ground-state density of the Moshinsky atom has the form \[ 11 \]

\[ \rho(r) = a \exp \left( -br^2 \right), \]  

(37)

where

\[ a = 2 \left( \frac{b}{\pi} \right)^{3/2}, \]  

(38)

\[ b = \frac{2\alpha - 1}{\alpha} \]  

(39)

and

\[ \alpha = \frac{1}{2} \left( 1 + (1 + 2K)^{1/2} \right). \]  

(40)

From Eqs. (1), (3), (4), and (37) we arrive at the expression

\[ S + \ln D = \frac{3}{2} (1 - \ln 2). \]  

(41)

Consequently, the complexity of the Moshinsky atom in the ground state is

\[ C_{LMC} = e^{\frac{3}{2}(1-\ln 2)}. \]  

(42)

This is again remarkable as it is a constant, independent of the coupling constant. In all the analytical results treated in this section, the parameter-free result for \( C_{LMC} \) is consequence of the homogeneous property of the corresponding potential. This has been
proven earlier in the cases of the composite information measures [12] and for complexity [6]. When the homogeneous property of the potential is lost, for example, under the confined conditions as we shall see in the next section, the $C_{LMC}$ values become dependent on some parameter of the potential.

IV. NUMERICAL RESULTS ON CONFINED MODEL SYSTEMS

The spherically confined Coulomb potential was originally introduced [4] in order to study the effects of high pressure on the dipole polarizability of hydrogen atom. In this model, the confining potential is defined in terms of an impenetrable spherical cavity of a certain radius of confinement, $R$. The spherically confined Coulomb potential for hydrogen-like atoms, for example, is given by

$$V(r) = -\frac{Z}{r} \quad \text{for} \quad r < R,$$
$$= \infty \quad \text{for} \quad r \geq R.$$  \hspace{1cm} (43)

We have carried out the calculations of $C_{LMC}$ corresponding to the following spherically confined model systems (a) particle in a spherical box (PIASB) (b)spherically confined isotropic harmonic oscillator (SCIHO), (c)spherically confined hydrogen atom (SCHA), all in position and momentum space and the two electron systems of (d) a pair of electrons and (e) He atom in position space. For the two electron systems we have employed the accurate 23-term and 70-term Hylleraas wave functions for the (d) and (e) cases, respectively. The numerical procedure adopted by us has been described in the literature [5, 6, 7] and will not be repeated here. Our results on the calculations of $C_{LMC}$ for systems (a)-(d) as a function of the radius of confinement, $R$, are displayed in Fig. 1.

For the PIASB cases (position and momentum space), the homogeneous character of the potential leads to a constant value of $C_{LMC}$ [6, 12]. In all other cases, the absence of homogeneous property of the potential gives rise to a nonlinear dependence of $C_{LMC}$ with $R$. The range of confinements considered by us presents a good test of the lower bound on $C_{LMC}$ obtained in Eq.(9). As is evident from Fig. 1, this bound is obeyed for all $R$ values across a diverse set of quantum confined systems. The general lower bound on $C_{LMC}$
derived in the present work is a significant addition to the characteristics of this statistical measure.

V. CONCLUSIONS

In summary, we derived a general lower bound for the shape complexity measure of Lopez et al. [1, 9] We also calculated the LMC measure for simple model systems: the harmonic oscillator, the hydrogen atom and two-electron ‘entangled artificial’ atom proposed by Moshinsky. We obtained the remarkable result that the LMC measure is constant, that is, it does not depend on any parameter. This is characteristic of the homogeneous property of the corresponding potentials. A representative set of confined Coulomb potentials have been used to numerically test the general validity of the lower bound obtained on $C_{LMC}$. Due to the non-homogeneous property of the potentials in these cases, $C_{LMC}$ becomes dependent on the parameters of the potential.

Acknowledgements

This work was written in the frame of the Bilateral Intergovermental Scientific and Technological Cooperation between Hungary and India sponsored by the Research an Technological Innovation Foundation and the Ministry of Science and Technology. ÁN acknowledges grant OTKA No. T67923. KDS is grateful to Jorge Garza and Rubicila Vargas for kind hospitality during the course of confined systems meeting held at UAM-I Mexico, in April 2009. We dedicate this work to the fond memory of Professor Marcos Moshinsky, UNAM, Mexico.
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FIG. 1: Variation of $C_{LMC}$ corresponding to the spherically confined model systems in position and momentum space for (a) particle in a spherical box (PIAB) (b) isotropic harmonic oscillator (SCIHO), (c) hydrogen atom (SCHA), and in position space for (d) a pair of electrons and (e) He atom. For (d) 23-term, and for (e) 70-term, Hylleraas wave functions have been employed.