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LMC complexity for the ground states of different quantum systems

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We dedicate this work to the fond memory of Professor Marcos Moshinsky, UNAM, Mexico.

ABSTRACT

Lower bound for the shape complexity measure of López-Ruiz–Mancini–Calbet (LMC), C_{LMC} is studied. 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.

1. 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 to consider the lower bound problem and the value of LMC complexity for the ground states of different quantum systems. 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 of one and two electron systems [4–7].

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

$$S_f=-\int f(\mathbf{r})\ln f(\mathbf{r})\,d\mathbf{r}, \tag{1}$$

$$H_f=e^{S_f}, \tag{2}$$

respectively. The so-called disequilibrium D has the form

$$D_f=\int f^2(\mathbf{r})\,d\mathbf{r}. \tag{3}$$

The definition of the continuous version of the LMC complexity measure is [9]

$$C_{\mathrm{LMC}}=H_f D_f \tag{4}$$

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.

2. Inequality for the LMC complexity

To derive a lower bound for the LMC complexity we cite Theorem 2 of the paper of Yáñez et al. [10]. The position-space entropy $\tilde{S}_\varrho$ of an N-electron system in a physical state characterized by the (normalized to N) one-electron density $\varrho(\mathbf{r})$ fulfills the inequality

$$\tilde{S}_\varrho+\langle\ln g(\mathbf{r})\rangle\leqslant N\ln\left(\frac{\int g(\mathbf{r})\,d\mathbf{r}}{N}\right), \tag{5}$$

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]:

$$S_f=\frac{\tilde{S}_\varrho}{N}+\ln N \tag{6}$$

and taking $g=f^2$, we obtain the inequality

$$S_f+\ln\left(\int f^2(\mathbf{r})\,d\mathbf{r}\right)\geqslant 0. \tag{7}$$

From the definition of the LMC complexity (4) we obtain the upper bound

$$\ln C_{\mathrm{LMC}}\geqslant 0 \tag{8}$$

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or

$$C_{\mathrm{LMC}} \geqslant 1. \tag{9}$$

As was rigorously proven in Ref. [9] the lower bound saturates in the rectangular probability distribution. 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.

3. 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

$$\psi_{e,n} = A\cos\left(\frac{n\pi x}{2a}\right), \tag{10}$$

if $|x| < a$. Odd solutions are

$$\psi_{o,n} = B\sin\left(\frac{n\pi x}{2a}\right), \tag{11}$$

if $|x| < a$. $n = 1, 2, \ldots,$ $A = B = 1/a^{1/2}$ is the normalization constant. The disequilibrium takes the form:

$$D = \frac{3}{4a} \tag{12}$$

for all eigenfunctions. The Shannon entropy can be written as

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

for the even solutions and

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

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

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

and

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

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. This result is closely related to the finding of López-Ruiz and Sañudo [11], that is, the complexity is constant for the whole energy spectrum of the d-dimensional quantum infinite square well.

It is possible to extend this result for the particle in a spherical box, PIASB represented by the radial Schrödinger equation

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

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

$$R_{nl} = N j_l(r\sqrt{2E}\,), \tag{18}$$

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 disequilibrium

$$D = \frac{Si(2\pi) - \frac{Si(4\pi)}{2}}{(r_c)^3} = \frac{0.6720709}{(r_c)^3}. \tag{19}$$

The Shannon entropy can be written as

$$S_r = \ln\left(8\pi r_c^3\right) - 3 + \frac{Si(2\pi)}{\pi}. \tag{20}$$

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

$$C_{\mathrm{LMC}} = 1.3207394, \tag{21}$$

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 $C_{\mathrm{LMC}} = 1.517215$.

As our second example, we consider free linear harmonic oscillator with potential $V = 1/2kx^2$. Then the ground-state density has the form

$$\varrho = \frac{k^{1/4}}{\pi^{1/2}} \exp\left(-k^{1/2}x^2\right). \tag{22}$$

We can immediately obtain the Shannon entropy:

$$S = -\ln\left(\frac{k^{1/4}}{\pi^{1/2}}\right) + \frac{1}{2} \tag{23}$$

and the disequilibrium:

$$D = \frac{k^{1/4}}{(2\pi)^{1/2}}. \tag{24}$$

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

$$\ln C_{\mathrm{LMC}} = S + \ln D = \frac{1}{2}(1 - \ln 2). \tag{25}$$

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

$$C_{\mathrm{LMC}} = e^{\frac{1}{2}(1-\ln 2)}. \tag{26}$$

This is a remarkable result as it is a constant, independent of k, as it has already been demonstrated by Sañudo and López-Ruiz [12].

The third example is the free hydrogen atom, or hydrogen-like atomic ions. The ground-state density takes the form

$$\varrho = \frac{Z^3}{\pi} \exp(-2Zr), \tag{27}$$

where Z is the atomic number. The Shannon entropy can be written as

$$S = 3 - \ln\left(\frac{Z^3}{\pi}\right), \tag{28}$$

while the disequilibrium takes the form:

$$D = \frac{Z^3}{8\pi}. \tag{29}$$

Eqs. (28) and (29) lead to the expression

$$\ln C_{\mathrm{LMC}} = S + \ln D = 3(1 - \ln 2), \tag{30}$$

so the complexity of hydrogen-like atomic ions in the ground state is