

Chapter 1

Information Planes for Complex Systems

P. Sánchez-Moreno

Departamento de Física Moderna & Instituto Carlos I (University
of Granada)

E. Romera

Departamento de Física Moderna & Instituto Carlos I (University
of Granada)

R.J. Yáñez

Departamento de Matemática aplicada & Instituto Carlos I
(University of Granada)

J.S. Dehesa

Departamento de Física Moderna & Instituto Carlos I (University
of Granada)

The concept of Fisher-Shannon information plane, defined by the Fisher information I and the Shannon entropy H of the one-particle distribution density, is proposed as a new tool to analyze the internal disorder of complex systems as well as to disentangle between their spectra regimes. The former is illustrated for various members of the He-like isoelectronic sequence, and the latter for the complex systems with a level spacings distribution of Berry-Robnik type.

1.1 Introduction

The Fisher information I and the Shannon entropy H measures of a D -dimensional random variable X whose probability density function is denoted as $\rho(\mathbf{x})$ were introduced by R.A. Fisher [3] in 1925 and C.E. Shannon [11, 12] in

1948 in the contexts of statistical estimation and communication engineering.

They are defined by

$$I_X = \int_{\Omega} \frac{(\vec{\nabla} \rho(\mathbf{x}))^2}{\rho(\mathbf{x})} d\mathbf{x} \quad (1.1)$$

for the Fisher information, and

$$H_X = - \int_{\Omega} \rho(\mathbf{x}) \log \rho(\mathbf{x}) d\mathbf{x} \quad (1.2)$$

for the Shannon entropy, respectively; Ω being the support of the density. For convenience the alternative notion of entropy power

$$N_X = \frac{1}{2\pi e} \exp\left(\frac{2}{D} H_X\right) \quad (1.3)$$

will be used rather than the entropy H_X .

Nowadays the Fisher and Shannon measures are being applied in numerous scientific branches, particularly in theoretical physics [4–6].

They give complementary descriptions for the spatial delocalization of the probability density, providing quantitative local and global measures of the smoothness of that density, respectively.

These two measures, I_X and N_X , satisfy a number of interesting properties [2]. We would like to remark that they verify the uncertainty inequality [2, 8]

$$\frac{1}{D} N_X I_X \geq 1 \quad (1.4)$$

provided that the support Ω extends over the whole space. This shows that when one of the involved measures decreases near to zero, the other has to increase to a large value. Moreover, these two measures transform as

$$I_{aX} = a^{-2} I_X \quad , \quad N_{aX} = a^2 N_X \quad (1.5)$$

under scaling of the random variable X by a real scalar factor a , what indicates that they are homogeneous density functionals of degrees 2 and -2 respectively. Consequently, the information product $\mathcal{P} := \frac{1}{D} N_X I_X$ is invariant under this scaling transformation.

These two uncertainty and scaling properties clearly manifest that the Fisher information and the Shannon entropy power are indeed closely linked, so that the characterization of the physical phenomena described by the associated probability density X should be improved by the analysis of its location in the Fisher-versus-Shannon plane.

Recently, the applicability of this information plane has been suggested for the characterization of signals [14]. Here we show the applicability of this plane and the usefulness of the new measure \mathcal{P} in two different directions. First, to explore the electron correlation in atomic and molecular systems by means of the proposal of a new correlation measure $\mathcal{P} = \frac{1}{3} I N$, where I and N represent

the Fisher information and Shannon entropy power of the electron distribution density of these systems, which complementarily and quantitatively measure the spatial delocalization of the electronic cloud, so the internal disorder of the systems. This is done for the ground-state of various He-like ions by use of the 204-terms Hylleraas-type functions [7], with and without electron-electron repulsion. Second, to distinguish between the regular and irregular spectral regimes of those complex systems characterized by an eigenvalue distribution of Berry-Robnik type [1, 13].

1.2 The Fisher-Shannon plane in electronic systems.

To exemplify the applicability of the Fisher-Shannon plane to explore the correlation properties of many-electron systems, we will consider the ground-state information plane of various two-electron systems with and without the electron-electron interaction, namely the ions H^- , He , Li^+ , Be^{2+} , Be^{3+} and Ne^{8+} which have a nuclear charge $Z = 1-5$ and 10 , respectively. The Hamiltonian of these systems is given by

$$H = \sum_{i=1}^2 \left(-\frac{1}{2} \nabla_i^2 + \frac{Z}{r_i} \right) + V_{ee}(\mathbf{r}_1, \mathbf{r}_2), \quad (1.6)$$

where $V_{ee} = 1/|\mathbf{r}_1 - \mathbf{r}_2|$ is the electron-electron repulsion. Atomic units are used in this section.

We have calculated the Fisher information and the Shannon entropy power for the aforementioned ions as well as for the bare-Coulomb-field case (i.e. without the electron-electron repulsion) [10]. For the latter case, the electron density is hydrogenlike so that $I = I(Z) = 4Z^2$ and $N = N(Z) = (2/2\pi^{1/3})Z^{-2}$; then the associated information product $\mathcal{P}(Z) = \frac{1}{3}I(Z)N(Z) \simeq 1.237333\dots = K_{BCF}$.

Let us now include the electron-electron repulsion V_{ee} , and let us compute the corresponding information measures by use of the 204-terms Hylleraas-type wavefunctions of Koga et al. [7]. The comparison of the computed results with the corresponding bare values are given in Fig. 1.1 and Fig. 1.2 for the Fisher-Shannon plane and the information product $\mathcal{P}(Z)$, respectively.

In Fig. 1.1 the area below the solid line (i.e. the line where $\mathcal{P}(Z) = 1$) cannot be spanned by any electron density. The dotted line, which corresponds to the bare case $\mathcal{P}(Z) = K_{BCF}$, include the bare He-like ions above mentioned. The crosses and the bullets correspond to the (N, I) values with and without the electron-electron repulsion, respectively. The crosses, as well as the bullets, correspond from the left to the right to increasing values of Z .

Some observations may be done. First, the crosses follow a Fisher-Shannon trajectory which depends on Z so that the information product $\mathcal{P}(Z)$ tends towards the bare Coulomb value K_{BCF} when the nuclear charge is increased. Second, the crosses are separated out from the dotted, no-correlation line; this

separation rapidly decreases when Z is increased. Third, for a given ion the cross is located higher and more to the left than the corresponding bullet, what indicates that the correlated value for the entropy power (Fisher information) is higher (lower) than the corresponding bare-Coulomb-field values. This is a clear evidence that the electron correlation produces a spreading effect in the electronic cloud, so increasing the internal disorder of the system. Fourth, the distance between the cross and the bullet of a given ion decreases very fast when Z is increased. The second and fourth observations show the known phenomenon according to which the aforementioned correlation spreading effect gradually decreases, and the ratio of the electron-electron and electron-nucleus strengths becomes very small, when Z is raised.

The first observation is a clear manifestation of the electron correlation in the information product. This can be also seen more in detail in Fig. 1.2, where we have plotted the dependence of this product on the nuclear charge for the He-like ions considered in this paper and for the bare two-electron atoms. Therein one notices again the monotonic decrease of the information product \mathcal{P} when Z is increased, asymptotically approaching the bare value K_{BCF} and showing that the electron correlation effect gradually decreases with respect to the electron-nucleus interaction when the nuclear charge of the system is raised.

1.3 The Fisher-Shannon plane for Berry-Robnik spectra.

The semiclassical spectrum of quantum complex systems may be characterized by means of the probability distribution $\rho(x)$ of the spacings x between successive energy levels. It is well-known that for integrable systems the levels are uncorrelated (regular regime), so that the level spacings distribution is of Poisson type, i.e.

$$\rho_P(x) = a_1 e^{-a_1 x} \quad (1.7)$$

where a_1 denotes the mean level density [1]. On the other hand, for non-integrable systems there often exists a repulsion phenomenon between adjacent levels so that the level spacings distribution has the Wigner form (see e.g. [9]),

$$\rho_W(x) = \frac{\pi}{2} a_2^2 x e^{-\frac{\pi}{4} a_2^2 x^2} \quad (1.8)$$

where a_2 represents the mean level density of this irregular regime.

Generic systems, however, often have a spectrum with both types of spectral regimes which at times are uncorrelated. Then, taking into account that the total level density $a_1 + a_2$ can be normalized to one, M.V. Berry and M. Robnik [1] have shown that the level spacings distribution is approximately given by

$$\rho_{BR}(x) = \left[(1 - \nu)^2 \operatorname{erfc} \left(\frac{\sqrt{\pi}}{2} \nu x \right) + \left(2\nu(1 - \nu) + \frac{\pi}{2} \nu^3 x \right) e^{-\frac{\pi}{4} \nu^2 x^2} \right] e^{-(1-\nu)x} \quad (1.9)$$

where ν gives the mean level density for the irregular region, and $1 - \nu$ is the corresponding quantity for the regular region. Remark that the limits $\nu = 0$ and $\nu = 1$ correspond to the Poisson and Wigner distributions, respectively. The Berry-Robnik distribution is plotted for these limits and for the values $\nu = 0.5$ and 0.7 in Fig. 1.3 to make clearer our discussion.

Here we will study the Berry-Robnik distribution from an information-theoretic standpoint. First, we have calculated the Fisher information of this distribution as a function of the parameter ν . The computed results are shown in Fig. 1.4, where we observe that this quantity has a quasiconstant behaviour for all values of ν between 0 (pure Poisson regime) up to ~ 0.7 , and then it rapidly increases when approaching $\nu = 1$ (pure Wigner regime). Then, we have calculated the Shannon entropy power as shown in Fig. 1.5. In contrast to the previous situation, we notice that the entropy power monotonically decreases from ~ 0.43 down to ~ 0.25 when ν varies within the interval $[0, 1]$, i.e. when the system goes from the regular to the irregular regime. This can be understood because in doing this transition the system becomes more constrained, what produces a more correlated spectrum, thus an enhancement of the order in the level spacings distribution which plausibly means a lower entropy power.

In addition we have plotted in Fig. 1.6 the information product NI in terms of the parameter ν . Here again we observe the quasiconstant behaviour already noticed for the Fisher information, due to the fact that the range of variation of the entropy power values is not too big. Both Fig. 1.4 and Fig. 1.6 clearly indicate that the Fisher information as well as the information product NI are appropriate integrability measures of complex systems.

For completeness we have examined the Heisenberg-Shannon information plane for the Berry-Robnik distribution (1.9) which is the plane conformed by the variance σ^2 versus the reciprocal of the entropy power N of this distribution. It is shown in Fig. 1.7. Therein we observe that both the variance and the entropy power have a smooth decreasing behaviour, as a clear evidence of the transition from integrable to nonintegrable systems. This means from a spectral point of view the transition from the regular to the irregular regimes.

1.4 Conclusion.

We have shown the applicability of the concept of information plane to explore the complexity character of quantum systems. This has been exemplified in atomic systems where the Fisher-Shannon plane has been shown to illustrate the correlation phenomenon of the Helium-like systems. We have suggested the use of a new correlation measure defined by the product of the Fisher information and the Shannon entropy power. In addition, we have shown that this information product, as well as the Fisher quantity, may be used as nonintegrability measures of complex systems. Furthermore, other information planes as that of Heisenberg-Shannon may be used for similar purposes. In conclusion, we believe that the information plane is a very useful tool to explore the physical complexity of natural systems.

Bibliography

- [1] BERRY, M.V., and M. ROBNIK, “Semiclassical level spacings when regular and chaotic orbits coexist”, *J. Phys. A* **17** (1984), 2413–2421.
- [2] DEMBO, Amir, and Thomas M. COVER, “Information theoretic inequalities”, *IEEE Transactions on Information Theory* **37** (1991), 1501–1518.
- [3] FISHER, R.A., “Theory of statistical estimation”, *Proc. Camb. Phil. Soc.* **22** (1925), 700–725.
- [4] FRIEDEN, B.R., *Science from Fisher’s information*, Cambridge University Press (2004).
- [5] GONZÁLEZ-FÉREZ, R., and J.S. DEHESA, “Shannon entropy as an indicator of atomic avoided crossings in strong parallel magnetic fields”, *Physical Review Letters* **91** (2003), 113001–(1–4).
- [6] JAYNES, E.T., “Information theory and statistical mechanics i and ii”, *Phys. Rev.* **106** (1957), 620–630.
- [7] KOGA, T., Y. KASAI, and A.J. THAKKAR, “Accurate algebraic densities and intracules for helium-like ions”, *Int. J. Quantum Chem.* **46** (1993), 689.
- [8] PEARSON, J. Michael, “A logarithmic sobolev inequality on the real line”, *Proc. Amer. Math. Soc.* **125** (1997), 3339–3345.
- [9] PECHUKAS, Philip, “Distribution of energy eigenvalues in the irregular spectrum”, *Phys. Rev. Lett.* **51** (1983), 943–946.
- [10] ROMERA, Elvira, and J.S. DEHESA, “The fisher-shannon information plane, an electron correlation tool”, *Journal of Chemical Physics* **120** (2004).
- [11] SHANNON, C.E., “A mathematical theory of communication”, *Bell Syst. Tech. J.* **27** (1948), 623–656.
- [12] SHANNON, C.E., and W. WEAVER, *The Mathematical Theory of Communication*, University of Illinois Press (1949).
- [13] STÖCKMANN, H.-J., *Quantum Chaos, an introduction*, Cambridge University Press (1999).
- [14] VIGNAT, C., and J.-F. BERCHER, “Analysis of signals in the fisher-shannon information plane”, *Phys. Lett. A* **312** (2003), 27–33.

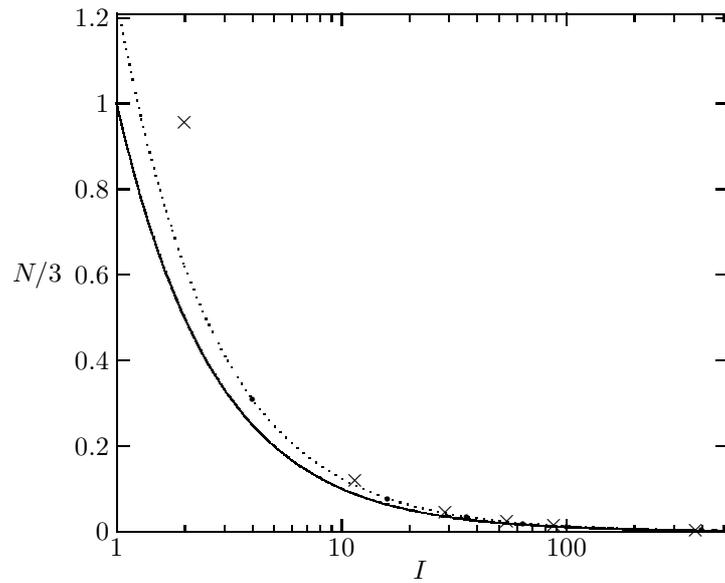


Figure 1.1: The Fisher-Shannon information plane of the He-like ions. Logarithmic scale is used for the Fisher information I . The crosses (\times) correspond to the ions with nuclear charge $Z = 1 - 5$ and 10. The solid line, which corresponds to $\mathcal{P} = \frac{1}{3}NI = 1$, is the borderline for the area of the points (I, N) which cannot be spanned by any electron density. The bullets (\bullet) on the dotted line (i.e. the set of points defined by $\mathcal{P} = K_{BCF}$; see text) correspond to the values (I, N) of the bare He(Z) ions with $Z = 1 - 5$ and 10.

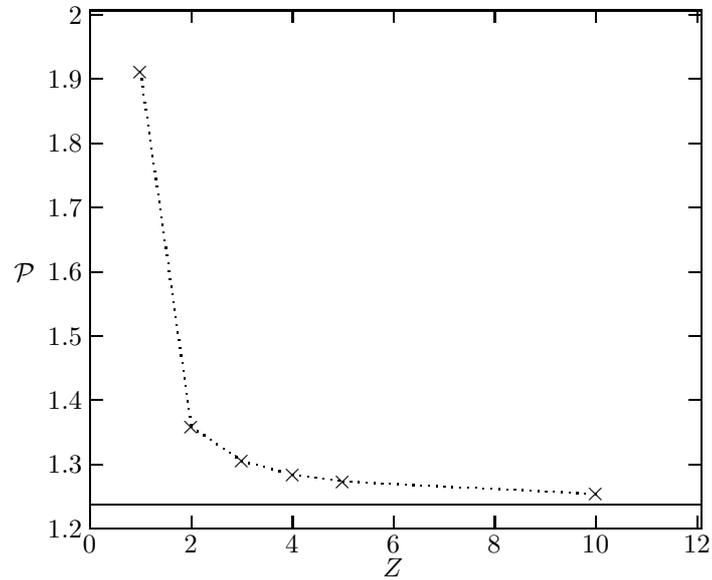


Figure 1.2: The information product $\mathcal{P} = \frac{1}{3}NI$ of the He-like ions and bare two-electron atoms as a function of the nuclear charge Z . The crosses correspond to the values of $\text{He}(Z)$ ions with $Z = 1 - 5$ and 10. The dotted line (...) has been drawn only to guide the eye. The solid straight line joins the points of the bare $\text{He}(Z)$ systems.

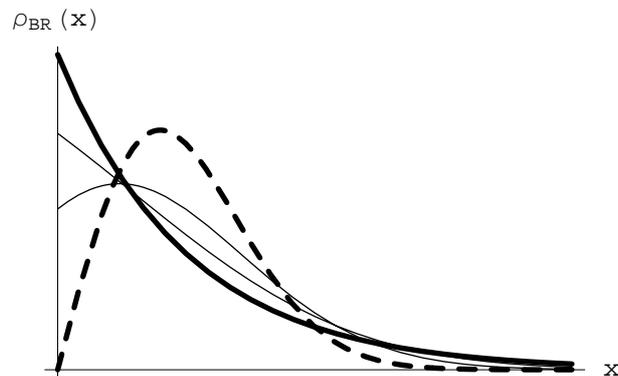


Figure 1.3: Berry-Robnik distribution. Thick solid line: $\nu = 0$ (Poisson), slim lines: $\nu = 0.5$ and $\nu = 0.7$, thick dashed line: $\nu = 1$ (Wigner).

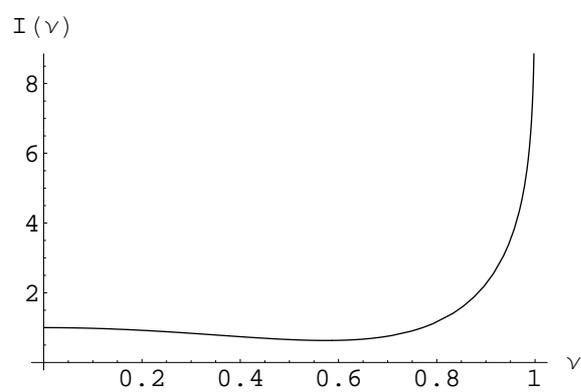


Figure 1.4: Fisher information for the Berry-Robnik distribution.

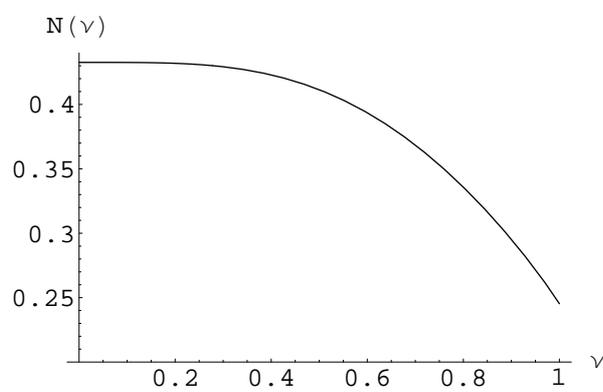


Figure 1.5: Entropy power for the Berry-Robnik distribution.

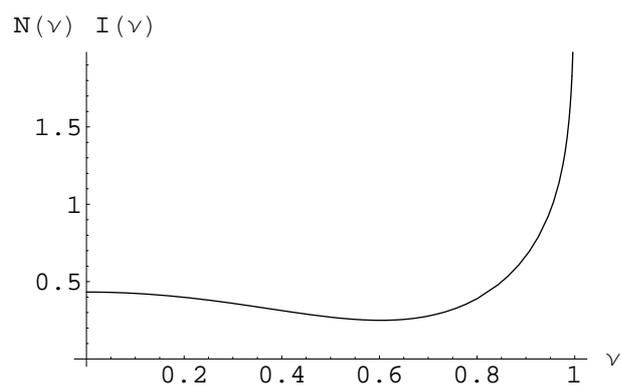


Figure 1.6: Information product for the Berry-Robnik distribution.

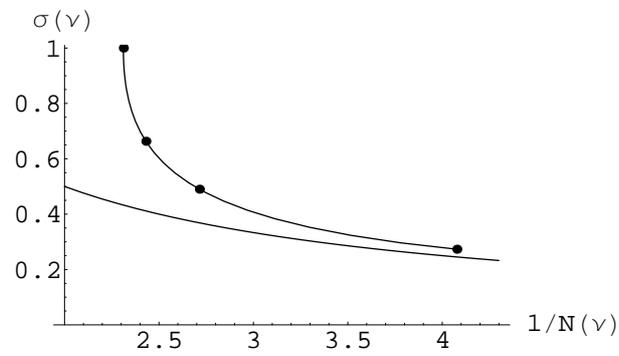


Figure 1.7: Heisenberg-Shannon information plane. From left to right, dots in curve correspond to $\nu = 0, 0.5, 0.7, 1$. Lower curve is part of the $\sigma^2/N = 1$ rectangular hyperbola.