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Statistical quantifiers for few-fermion' systems

F. Pennini [a,b,*], A. Plastino [c,d]

[a] Departamento de Física, Universidad Católica del Norte, Av. Angamos 0610, Antofagasta, Chile
[b] Departamento de Física, Facultad de Ciencias Exactas y Naturales, Universidad Nacional de La Pampa, CONICET, Av. Peru 151, 6300, Santa Rosa, La Pampa, Argentina
[c] Instituto de Física La Plata-CCT-CONICET, Universidad Nacional de La Plata, C.C. 727, 1900, La Plata, Argentina
[d] SThAR-EPFL, Lausanne, Switzerland

HIGHLIGHTS

- Exactly solvable few-fermion systems are discussed at finite temperature.
- The behavior of statistical quantifiers is investigated.
- The statistical complexity is assessed with the same criteria in large systems and for few-fermions.
- At finite temperature, remnants of phase transitions' remain.

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ABSTRACT

With reference to a simple (analytically solvable) model containing a few fermions, we show that statistical quantifiers, devised for large numbers of particles (and macroscopic bodies), surprisingly turn out to provide significant insights into the fermion-model characteristics. We find that statistical complexity can be assessed with the same criteria in large systems and in few-fermions ones.

1. Introduction

Knowledge regarding a system's unpredictability/randomness does not suffice for a proper grasping of the extant correlation structures. One may long for the possibility of being in a position to get insight into the relations amongst a system's components via an adequate quantifier, in a manner similar to that in which entropy S captures disorder. Two extreme situations exist: (1) Perfect order or (2) maximal randomness. These are not endowed with strong correlations [1]. Between them different degrees of correlation could exist. A quantifier reasonably called complexity might be needed. The question how is to represent it. The response is not easy to formulate. Famously, Seth Lloyd listed about 40 ways of defining a complexity, none of them quite satisfactory.

Obviously, a system may be deemed complex when it does not fit patterns viewed as simple. Think of (1) a perfect crystal and (2) the isolated ideal gas as adequate examples of simplicity, i.e., instances of vanishing complexity. The first is totally ordered and the second totally random. Little information suffices to describe the perfect crystal: the distances and the symmetries that define the elementary cell. The information, or negentropy ($-S$), stored in this system can be considered

* Corresponding author at: Departamento de Física, Universidad Católica del Norte, Av. Angamos 0610, Antofagasta, Chile.
E-mail address: fpennini@ucn.cl (F. Pennini).

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minimal. Instead, the isolated ideal gas is completely disordered. The system can be found in any of its accessible states with the same probability. All its degrees of freedom contribute in equal measure to the information contained in the ideal gas, that exhibits a maximum entropy. Systems (1) and (2) are extreme in the scale of order and information. This suggests that complexity should not be expressed just in terms of order or information. One could plausibly advance a measure of complexity by employing some kind of distance to the uniform distribution of accessible states. This is called disequilibrium (D) in the literature [2].

In this manner, D would yield a notion of probabilistic hierarchy. It would be different from zero if there are privileged, or more probable, states among those accessible. This by itself is not enough. D would be maximal for the perfect crystal. For the ideal gas, $D = 0$. Now, for entropy (S), matters are exactly reversed S is minimal for the crystal and maximal for the ideal gas. Such considerations led L. Ruiz, Mancini, and Calvet (LMC) [1] to propose a statistical complexity measure C of the form $C = DS$, a proposal that received much attention and interest [1,3–9]. It is clear that C vanishes in the (opposite) simple cases (1) and (2) above.

We will here show that quantifiers like S, D, and C, do yield important information regarding the behavior of a simple, few-fermions system.

2. The model

The Lipkin Model [10] has been shown to be very useful in studies concerning the validity and/or usefulness of variegated theoretical approaches, created so as to investigate the manifold aspects of the fermionic many body problem. This model is grounded on the SU(2) algebra and yields readily available exact solutions, which are to be compared vis a vis results gotten by recourse to different kinds of approximations. Here we consider a simplified version of that model, advanced in Ref. [11].

The two models (discussed in Refs. [10,11]) consist of N fermions distributed between ($2N$)-fold degenerate single-particle (sp) levels, separated by a sp energy gap ϵ. Two quantum numbers are associated to a generic single particle state. One of them adopts the values $\mu = -1$ (lower level) and $\mu = +1$ (upper level). The other quantum number, let us denote it by p, usually called quasi-spin or pseudo spin, singles out a state within the N-fold degeneracy. The pair $p,\ \mu$ can also be regarded as a site that is occupied or empty. In this model one has

$$N = 2J, \tag{1}$$

with J denoting an "angular momentum". Following Lipkin et al. [10] we introduce the well known quasi-spin operators

$$\hat{J}_+ = \sum_p C^\dagger_{p,+} C_{p,-}, \tag{2}$$

$$\hat{J}_- = \sum_p C^\dagger_{p,-} C_{p,+}, \tag{3}$$

$$\hat{J}_z = \sum_{p,\mu} \mu\, C^\dagger_{p,\mu} C_{p,\mu}, \tag{4}$$

$$\hat{J}^2 = \hat{J}_z^2 + \frac{1}{2}(\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+), \tag{5}$$

where the eigenvalues of $\hat{J}^2$ are of the form $J(J+1)$.

Our Hamiltonian is not that of Ref. [10] but that of reference [11], that reads

$$\hat{H} = \epsilon\hat{J}_z - V_s\left(\frac{1}{2}(\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+) - \hat{J}\right), \tag{6}$$

or, with $V = V_s/\epsilon$, or $\epsilon = 1$,

$$\hat{H} = \hat{J}_z - V\left(\frac{1}{2}(\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+) - \hat{J}\right), \tag{7}$$

so that the unperturbed ground state ($V = 0$) becomes, according to Eq. (1),

$$|J, J_z\rangle = |J, -N/2\rangle, \tag{8}$$

with energy

$$E_o = -N/2. \tag{9}$$

Doubly occupied p-sites are not permitted. It is clear that our Hamiltonian also commutes with the two operators $\hat{J}^2$ and $\hat{J}_z$. Hence, the exact solution will belong to the J-multiplet of the unperturbed ground state, whose states we will here from denote as $|J, M\rangle$. One of these states will minimize the energy. The pertinent M value depends upon the strength V of the interaction. We just saw that for the unperturbed ground state (ugs) we have $M = -J = -N/2$. Clearly, $(\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+)$ is a quasi-spin flipping operator. Accordingly, it becomes the more effective the more balanced the populations of the two-levels are.

2.1. Phase-transitions at zero temperature

The interesting feature of this model is that, as V grows from zero, E_o is not immediately affected. It keeps it value until a critical V-special value is reached, of $1/(N-1)$. At this stage, the interacting ground state suddenly becomes $|J, -N/2+1\rangle$. If V keeps growing, additional phase transitions ensue. The phase transition between $J_z = -k$ and $J_z = -k+1$ occurs at $V = 1/(2k-1)$ and the process ends when we reach either $J_z = 0$ ($V_{crit} = 1$ for integer J), or $J_z = -1/2$ ($V_{crit} = 1/2$ for odd J). Thus, at such stage we have, independently of J [11]:

$$V_{crit} = 1/2 \text{ for half} - \text{integer} J \text{ or } \; V_{crit} = 1 \text{ for integer} J. \tag{10}$$

3. Statistical treatment at finite temperature *T*

This is rather simple in this model because double occupancy of a p-site is forbidden. As a consequence, the Hamiltonian matrix is just the $(2J+1)\times(2J+1)$ one of the $J_z = -N/2$ multiplet, since the only way to get different J's to that above is to have double occupancy [12].

The $J = N/2$ multiplet is the only one considered by Lipkin et al. in their pioneer, original paper [10]. Of course, also by us here. Why? The reason lies in the nature of the respective Hamiltonians H. In all other multiplets, one encounters paired particles that simultaneously occupy the same site in both upper and lover levels. In order to specify the microstates taking into account these paired states one needs an additional quantum number called the quasi-spin seniority s [12]. For our $J = N/2$ multiplet we have $s = 0$. Our present Hamiltonian cannot see these paired particles and cannot connect states with different s (the pertinent matrix element vanishes). If there are paired sites, effectively, one would be dealing with $N - 2s$ particles (is there are s paired sites) and not with N ones. The other multiplets become relevant only if pairing forces are included in H [12], which we intend to do in future research. Remember that our present goal is to investigate statistical quantifiers in this environment, not the thermal analysis of the multiplet structure of the Lipkin model, that has been exhaustively examined many years ago (see, for instance, [13] and references therein).

One has for the free energy F and partition function Z, with β the inverse temperature,

$$F = -T\ln Z = -T\ln \mathrm{Tr}(\exp(-\beta\hat{H})), \tag{11}$$

where, hereafter, we set the Boltzmann constant $k_B = 1$.

Since J is fixed, because so is the particle number, in the Trace we sum over the J_z quantum number m. Given that H commutes with both J and J_z we get

$$Z = \sum_{m=-J}^{m=J} \exp(-\beta E_m), \tag{12}$$

with the energy E_m given by

$$E_m = m - V(J(J+1) - m^2 - J). \tag{13}$$

Note that the all important associated probabilities P_m are [14]

$$P_m = \frac{\exp(-\beta E_m)}{Z}, \tag{14}$$

for all $m = -J, -J+1, \ldots, J-1, J$. Also, the Boltzmann–Gibbs S entropy becomes

$$S = -\sum_{m=-J}^{m=J} P_m \ln P_m, \tag{15}$$

while the uniform probabilities are $P^{(u)} = 1/(2J+1)$ for all m. Finally, the LMC disequilibrium is [1]

$$D = \sum_{m=-J}^{m=J} (P_m - P^{(u)})^2. \tag{16}$$

For details, properties, and others applications of D, see Refs. [2,9]. We emphasize that LMC define the statistical complexity as [1]

$$C = S\,D. \tag{17}$$

3.1. Our goal

We wish to ascertain to what an extent the above statistical quantifiers are significant in providing information at finite temperature. In particular, we are interested in the phase transitions described above at zero temperature.

- Is this structure preserved at finite T (if T is low enough)?
- Is such a fact made evident by our quantifiers?
- What are low (or too high) temperatures?

We will show below that $\beta < 1$ (arbitrary units) entails high temperature and vice versa.

4. Results and discussions

4.1. Limit $t \to \infty$

The red curves in all Figs. 3–5 are easily obtained. Let us set $\beta = 0$ in Eqs. (12) and (14). Then, we immediately get $Z = 2J + 1$ and $P^{(u)} = 1/(2J + 1)$ (the uniform distribution), so that appeal to Eqs. (16) and (17) yields, in this limit,

$$D = C = 0 \quad \text{for all } J, \tag{18}$$

as it should, and

$$S = \ln(2J + 1). \tag{19}$$

For example, for $J = 3/2$, in addition to relation (18), we also have: $Z = 4$, and $S = \ln 4 = 1.38$. This is illustrated by the red line in Fig. 3(a). The same procedure was used in Figs. 3–5.

4.2. Limit $T \to 0$

In this instance, $S = 0$ implying $C = 0$. For example, for $J = 3/2$, the corresponding probabilities of the multiplet are: $P_{1/2} = P_{3/2} = 0$, $P_{-3/2} = \Theta(1/2 - V)$, and $P_{-1/2} = 1 - P_{-3/2} = \Theta(V - 1/2)$, where $\Theta(x)$ is the step function, leading to $S = 0$. See Fig. 1 as an illustration.

4.3. General

We present below graphs for $\beta = 0, 2, 4, 6, 10, 20, 60$. Four instance are considered with regards to the fermion-number N. We consider $N = 3, 4, 5, 6$. We focus our results in: probabilities P_m, disequilibrium D, entropy S, and statistical complexity C.

Fig. 2 depicts, for J=3/2, P_m:m=$-3/2$, $-1/2$, versus the coupling constant V. It is apparent that these two probabilities cross at $V_{crit} = 1/2$. For the statistical pundit, this immediately entails that at *this* V-value the entropy will grow and the disequilibrium will diminish. Why? Entropy has been shown to be synonym of ignorance [15]. Here, we speak of ignorance regarding the state of the system, which clearly augments at an occupation-probability's level-crossing. On the other hand, disequilibrium is distance to the uniform probability, that obviously diminishes as two of the four probabilities P_m become equal.

All this is confirmed by Figs. 3(D), 4(S), and 5(C), which were obtained numerically using the definitions of the preceding Section. At $\beta = 60$ the phase transitions are clearly appreciated via these quantifiers. When the temperature grows, the quantum structure is destabilized and its $T-$ associated ravages become more and more noticeable, until vanishing for $\beta = 0$. Note that the statistical complexity exhibits structured peaks at the critical V's. At the top we appreciate two tiny sub-peaks and a small sub-valley. We confirm the notion that the system becomes complex only at the critical points. Summing up:

- Entropy S displays peaks at the V's critical values. These peaks become gradually attenuated as T grows, and eventually disappear.
- Disequilibrium D suddenly drops at the V's critical values, displaying sharp glens that become gradually attenuated as T grows, and eventually disappear.
- Statistical complexity displays structured peaks at the V's critical values, with sub-peaks just before and just after V_{crit} and a small fall at V_{crit}. These peaks become gradually attenuated as T grows, and eventually disappear. This is the signature of a complex process taking place at the critical coupling constant.
- The ordered nature of the model, which becomes complex just at the phase transitions, survives at finite temperature, but it is eventually killed at T high enough, as expected.

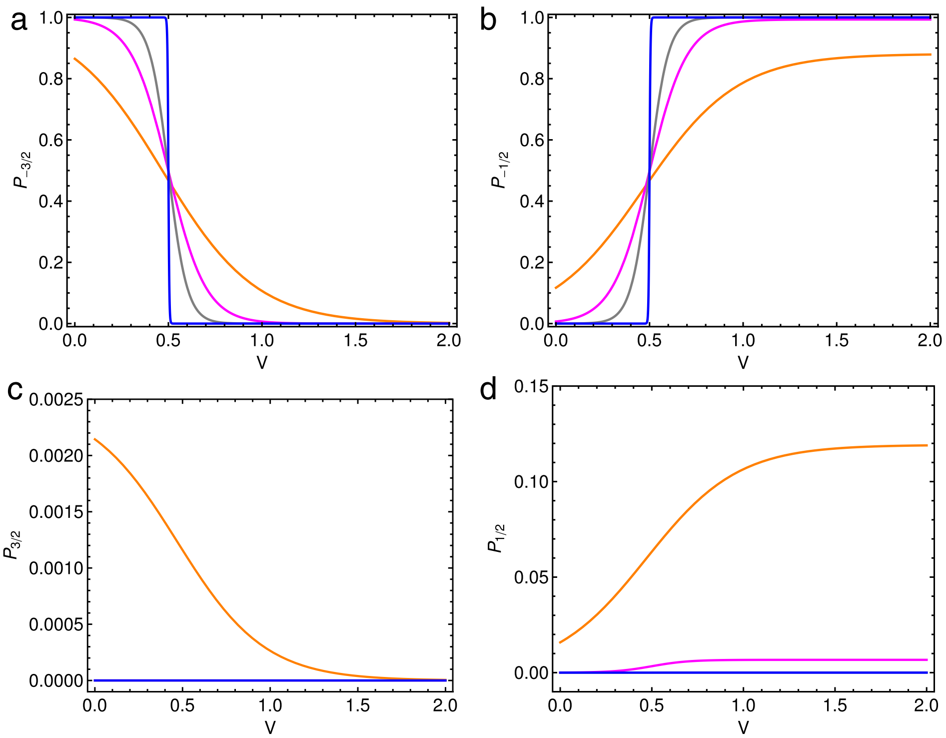

Fig. 1. Probabilities $P_{-3/2}$ in (a), $P_{-1/2}$ in (b), $P_{3/2}$ in (c), and $P_{1/2}$ in (d) as a function of V for $\beta = 2$ (orange curve), $\beta = 5$ (magenta curve), $\beta = 10$ (gray curve) and $\beta = \infty$ given by the step function $\Theta(1/2 - V)$ in (a) and $\Theta(V - 1/2)$ in (b) (blue curves). For $\beta = 10$, $P_{3/2}$ and $P_{1/2}$ are so small that cannot be seen in the figure's scale.

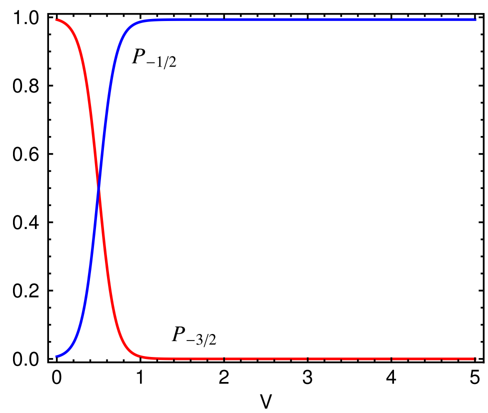

Fig. 2. Probabilities P_m as a function of V for $\beta = 5$ (arbitrary units) and $J = 3/2$. We have considered the cases $m = -3/2$ and $m = -1/2$. We observe that, at $V_{crit} = 1/2$, we find equal probabilities.

An important thing to be elucidated is: what temperatures are to be regarded high in this environment? An answer is provided by Eq. (10). In this model, the entropy is computed as a function of J, V, and β. Our tools are now density plots. In an S-density plot, we keep either J ($J = 1, 3/2, 2, 5/2, 3, 6$), or V constant and work on the plane of the other two quantities. We construct an S-estimate which reflects on the underlying probabilities. This gives the density according to which the S values (via the occupation probabilities) are distributed, the data being a random sample from those S-values.

Thus, we work on the first on the $J - \beta$-plane and then on the $V - \beta$-plane, which yields Figs. 6 and 7, respectively, as a density estimation for the entropy S. The clearer the color, the higher the density, or, in different words, the darker the color, the smaller the density.

Quantum effects are manifested by the peaks at $N = \text{odd}, \text{ even}$ (Fig. 6) or at $V = 1/2$ or $V = 1$ (Fig. 7), respectively (our phase transitions). They are clearly erased by temperature whenever $\beta \sim 2$. There, the peaks vanish. For larger β-values, the transitions-peaks of our model are easily seen. This entails low enough T.

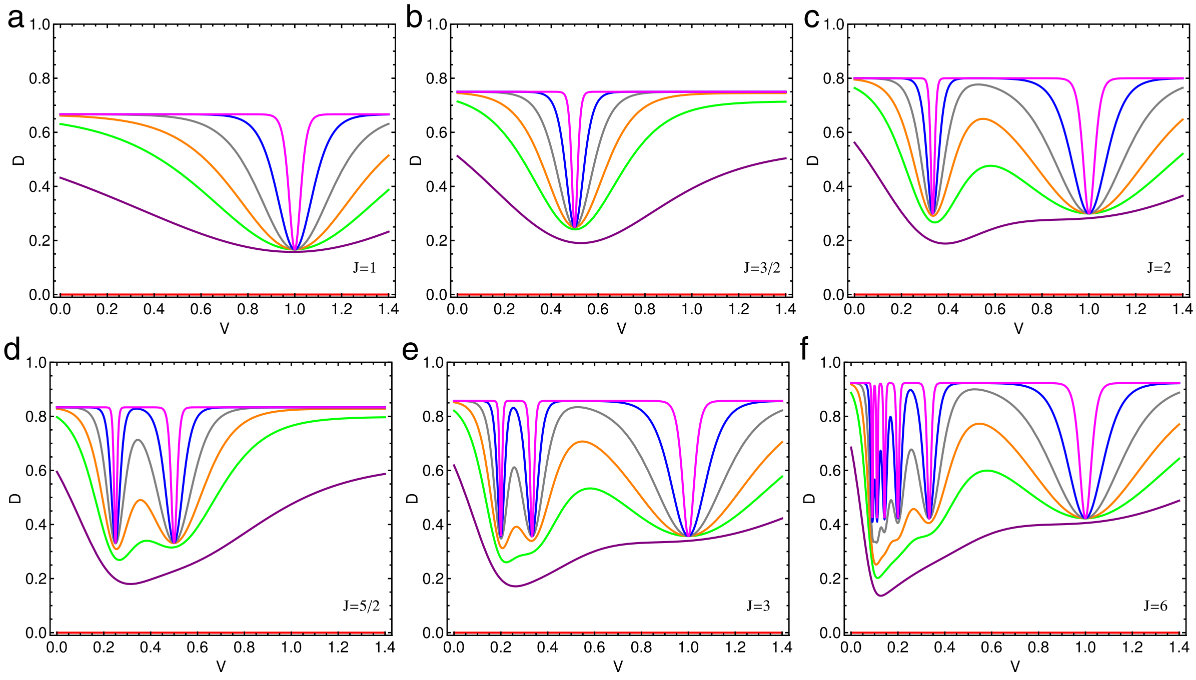

Fig. 3. Disequilibrium D as a function of coupling V for $\beta = 0$, 2, 4, 6, 10, 20, and 60 at different J's: (a) $J = 1$, (*b*) $J = 3/2$, (c) $J = 2$, (d) $J = 5/2$, (e) $J = 3$, and (f) J=6. The corresponding colors for curves are: $\beta = 0$ (red), 2 (purple), 4 (green), 6 (orange), 10 (gray), 20 (blue), while the magenta curve corresponds to $\beta = 60$.

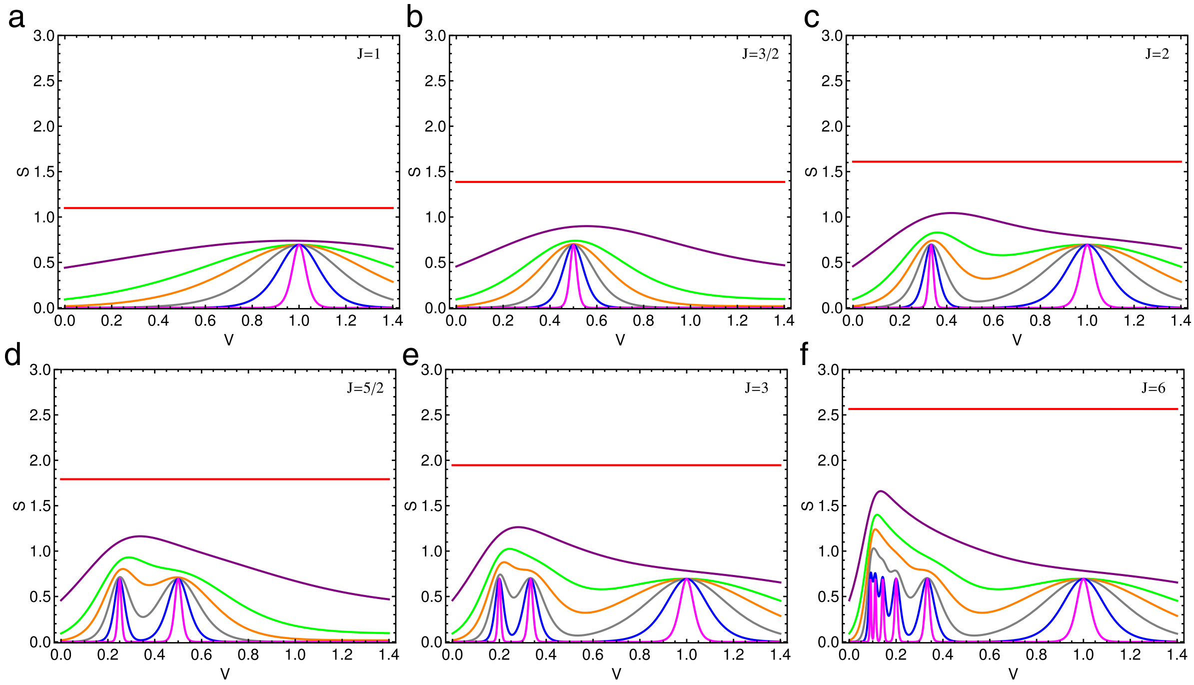

Fig. 4. Entropy S as a function of coupling V for $\beta = 0$, 2, 4, 6, 10, 20, and 60 at different J's: (a) $J = 1$, (*b*) $J = 3/2$, (c) $J = 2$, (d) $J = 5/2$, (e) $J = 3$, and (f) J=6. The corresponding colors for curves are: $\beta = 0$ (red), 2 (purple), 4 (green), 6 (orange), 10 (gray), 20 (blue), while the magenta curve corresponds to $\beta = 60$.

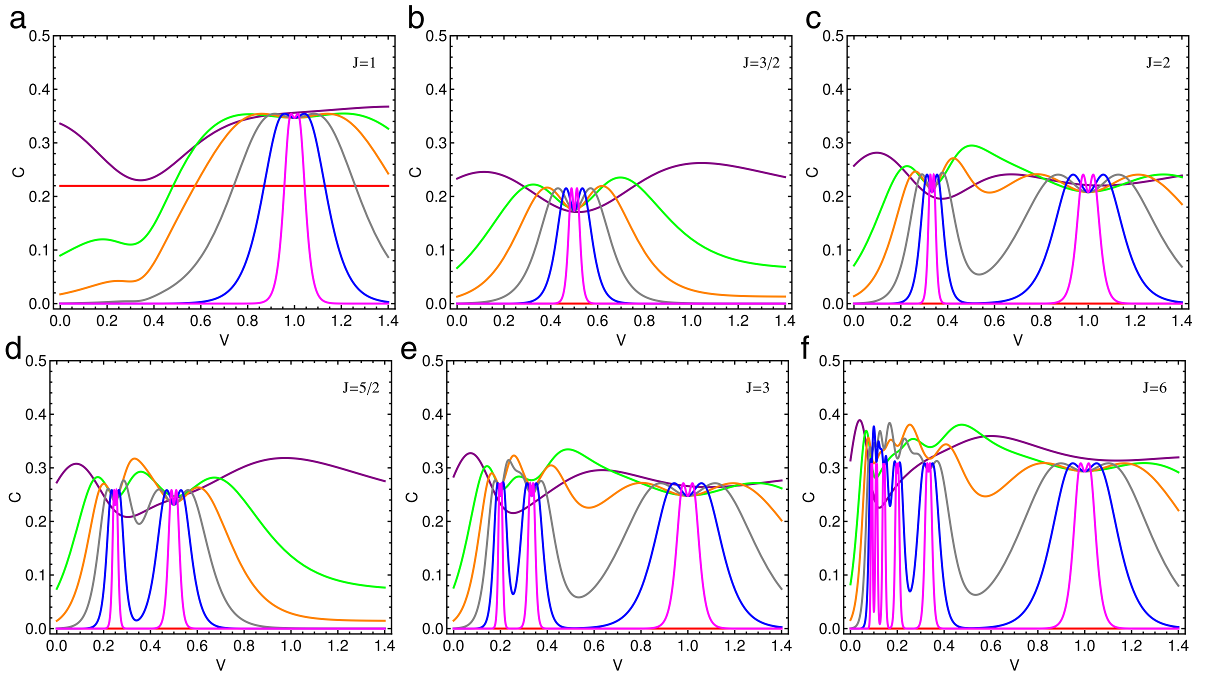

Fig. 5. Statistical complexity C as a function of coupling V for $\beta = 0, 2, 4, 6, 10, 20$, and 60 at different J's: (a) $J = 1$, (b) $J = 3/2$, (c) $J = 2$, (d) $J = 5/2$, (e) $J = 3$, and (f) J=6. The corresponding colors for curves are: $\beta = 0$ (red), 2 (purple), 4 (green), 6 (orange), 10 (gray), 20 (blue), while the magenta curve corresponds to $\beta = 60$.

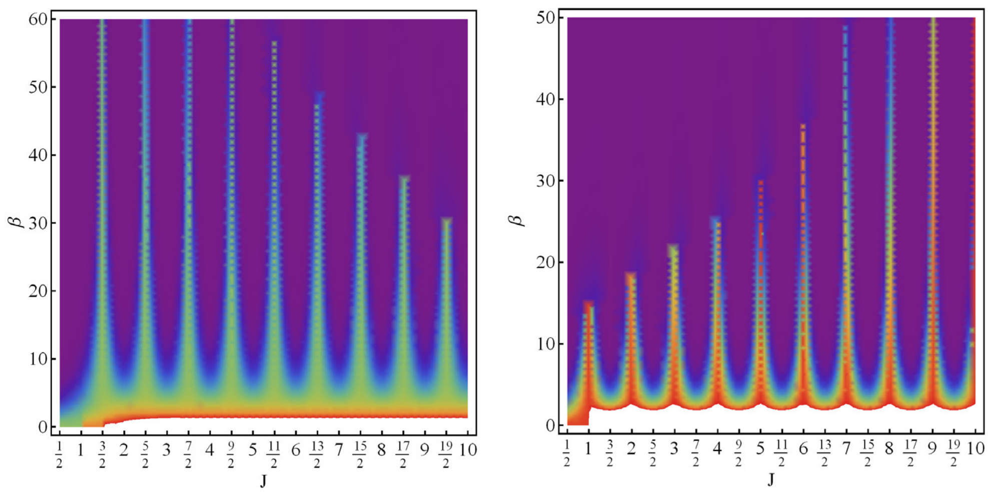

Fig. 6. Density plot of entropy S as a function of J and β for fixed V. To the left we find the figure corresponding to $V = 1/2$ and to the right that for $V = 1$.

5. Conclusions

We dealt with a simple, exactly solvable few-fermions system that exhibits phase transitions in the coupling constant. We have seen that such zero-temperature feature remains visible at finite temperatures, if T is not too high. How do they become visible? This the essence of our present contribution. They do so via statistical quantifiers devised for the macroscopic world, even if we face here just a few fermions. We found that statistical complexity can be successfully assessed with the same criteria in large systems (macroscopic bodies) and in few-fermions ones. We note that some statistical treatments of few nucleon systems have been reported in Ref. [16], unrelated to the present effort.

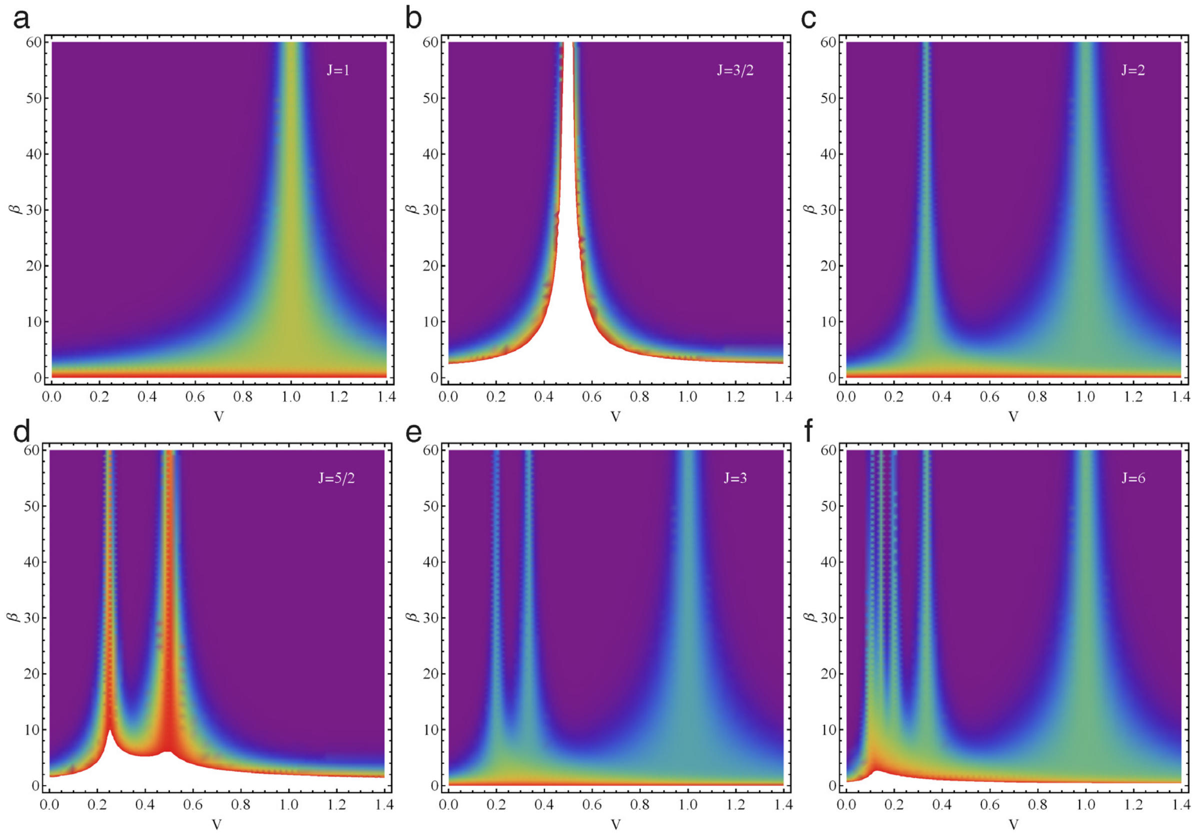

Fig. 7. Entropy S's density plot as a function of V and β for: (a) $J = 1$, (b) $J = 3/2$, (c) $J = 2$, (d) $J = 5/2$, (e) $J = 3$, and (f) $J = 6$.

Summing up, for macroscopic bodies we need classical probabilities. For fermionic systems, quantum ones. But in both situations we use probabilities in the same fashion, to obtain the statistical quantifiers S, D, and C, that do provide interesting insights into the system's nature.

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