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Spectral Explanation for Statistical Odd-Even Staggering in Few Fermions Systems

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Abstract: Odd-even statistical staggering in a Lipkin-like few fermions model has been recently encountered. Of course, staggering in nuclear binding energies is a well established fact. Similar effects are detected in other finite fermion systems as well, as for example, ultra small metallic grains and metal clusters. We work in this effort with the above-mentioned Lipkin-like, two-level fermion model and show that statistical staggering effects can be detailedly explained by recourse to a straightforward analysis of the associated energy-spectra.

Keywords: statistical complexity; exactly solvable models; even-odd effects

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1. Introduction

A well known fermion phenomenon is odd-even statistical staggering. It is found in few (not necessarily nuclear) fermion systems. The effect is empirically well known in nuclear physics and metal clusters ([1–3], and references therein). The associated odd-even differences in nuclear masses are also influenced by mean-field and odd-nucleon blocking effects [4,5].

We will deal below with an exactly solvable (interacting) fermions-model of the Lipkin kind that does not appeal to pairing interactions. This is relevant as paring forces are believed to be responsible for the effect in nuclei [3]. It was shown in [6] that odd-even differences are an intrinsic consequence of the dynamics of interacting fermions. The ensuing odd-even differences were incorporated [6] into an order–disorder environment that has as a protagonist the so-called statistical complexity concept [7], where "order" is produced by the fermion–fermion interaction while disorder is generated by the temperature T.

The above-mentioned order–disorder interplay was described in [6] via Gibbs' canonical ensemble considerations. In them, the concomitant probability distribution is proportional to $\exp(-\beta\hat{H})$, with $\hat{H}$ standing for the Hamiltonian and β for the inverse temperature.

We will see below that the staggering effect is translated from the energy (in the nuclear instance) to thermal quantifiers like the statistical complexity or the entropy. Interestingly enough, it manifests itself also in the variation of the mean energy with the temperatures, i.e., the specific heat.

More importantly, we will explicitly demonstrate that odd-even differences are entirely attributable to the characteristics of the associated energy-spectra of either odd or even systems.

2. The Model

The Lipkin Model (LM) [8] was very useful in research that revolved around the validity and/or usefulness of several theoretical techniques devised for investigating the multiple facets of the fermion many-body problem. The LM is based on an SU(2) algebra and produces easily accessible exact solutions.

We will occupy ourselves here with a simplified LM-version proposed in Reference [9].

The models of [8,9] deal with of N fermions distributed between (2N)-fold degenerate single-particle (sp) levels separated by an sp energy gap ϵ. Two quantum numbers (μ and p) are assigned to a general single sp. The first takes the values $\mu = -1$ (lower level) and $\mu = +1$ (upper level). The $p-$, often denominated quasi-spin or pseudo spin, picks out a specific belonging to the N-fold degeneracy. The couple p, μ may be viewed as a "site" that is occupied or empty. Double site-occupancy is forbidden. We have

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

where J stands for an "angular momentum". In the wake of Lipkin et al. [8] we define the 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 $J(J+1)$.

The model's Hamiltonian of Reference [9] is

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

Simplifyng with either $V = V_s/\epsilon$ or $\epsilon = 1$, we write

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

and the unperturbed ground state (gs) for $V = 0$ is, on account of Equation (1),

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

endowed with energy

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

The interaction between two fermions here is of a very simple nature. We have just forward scattering [9]. In interacting, the states of the two incoming fermions are identical to those of the two outgoing ones [9].

An important fact, we reiterate, is that doubly occupied $p-$sites are not allowed for. The Hamiltonian commutes with the pair of operators $\hat{J}^2$ and $\hat{J}_z$.

Accordingly, the exact solution must be encountered within the J-multiplet of the unperturbed ground state. The states of such multiplet will be denoted as $|J, M\rangle$. One of them has then to minimize the energy. The ensuing M value should depend on the strength V of the interaction.

A remarkable trait of our model [9] is that, as V increases from zero, E_o is not at once modified. It maintains its value till a critical $V-$specific figure is reached, of $1/(N-1)$. At this juncture, the interacting ground state abruptly becomes $|J, -N/2+1\rangle$. If V continues augmenting, additional "crossing" transitions (ct) take place (the J_z-value characterizing the ground state changes). The ct between $J_z = -k$ and $J_z = -k+1$ happens at $V = 1/(2k-1)$.

This ct-series ends as the interacting ground state becomes either $J_z = 0$ ($V_{crit} = 1$ for integer J), or $J_z = -1/2$ ($V_{crit} = 1/2$ for odd J). In such circumstances one has, regardless of the value J [9]

$$V_{crit} = 1/2, \tag{10}$$

for half-integer J and

$$V_{crit} = 1, \tag{11}$$

for integer J.

Our Model at Finite Temperatures

One needs to compare model-results for distinct J values, which is facilitated because double occupancy of a p-site is strictly forbidden. Accordingly, the Hamiltonian matrix should be the $(2J+1) \times (2J+1)$ one of the $J_z = -N/2$ multiplet, with $N = 2J$ [8].

One has for the free energy $F(J)$, in terms of the partition function $Z(J)$,

$$F = -T \ln Z = -T \ln \mathrm{Tr}(\exp(-\beta \hat{H})), \tag{12}$$

where, hereafter, we set the Boltzmann constant equal to unity. For each different J the trace operation is a sum over the J_z quantum number m and

$$Z(J) = \sum_{m=-J}^{m=J} \exp(-\beta E_m^J), \tag{13}$$

with an energy E_m^J [9]

$$E_m^J = m - V[J(J+1) - m^2 - J]. \tag{14}$$

The pertinent Gibbs' probabilities P_m^J then become [9]

$$P_m^J = \frac{\exp(-\beta E_m^J)}{Z(J)}, \tag{15}$$

for all $m = -J, -J+1, \ldots, J-1, J$. Thus, the Boltzmann–Gibbs S entropy is ([10] pp. 202–211)

$$S(J) = -\sum_{m=-J}^{m=J} P_m^J \ln P_m^J, \tag{16}$$

As for the number of micro-states m one has, of course,

$$O(J) = 2J + 1, \tag{17}$$

so that the pertinent uniform probabilities (the same for any m) should read

$$P(u_J) = 1/O(J). \tag{18}$$

3. LMC Statistical Complexity

This notion is of the essence here [7,11–24]. That of complexity is a pervasive notion in modern science. Any complex system is customarily linked with a mixture of order and disorder as well as to emergent phenomena. However, a universal and precise definition of complexity is still missing. There are different ways to calculate it, like the so-called algorithmic complexity, introduced by Kolmogorov so as to avoid the probabilistic interpretation of Shannon. Nevertheless, a successful and much utilized expression for it is that advanced by L. Ruiz, Mancini, and Calbet (LMC) [7] that we will employ in this work. Mathematically, it is the product of the ordinary entropy S times a distance in probability space between the current probability distribution and the uniform one. This distance is called the disequilibrium D. D is a measure of "order" as the larger it becomes, the larger the quantity of "privileged" states in our sample state's space (our J multiplet here). It is defined as [7]

$$D(J) = \sum_{m=-J}^{m=J} [P_m^J - P(u_J)]^2. \tag{19}$$

D tells us about the degree of "order" in our system. This order grows with D. To learn about more details, features, and applications of the disequilibrium the reader is directed to References [23,24]. We reiterate that LMC defines the statistical complexity C as [7],

$$C = S\,D. \tag{20}$$

In Reference [6], it was discovered that the three quantifiers (S, D, and C) display the odd-even effect. An example is displayed below in Figure 1, where it is clearly appreciated.

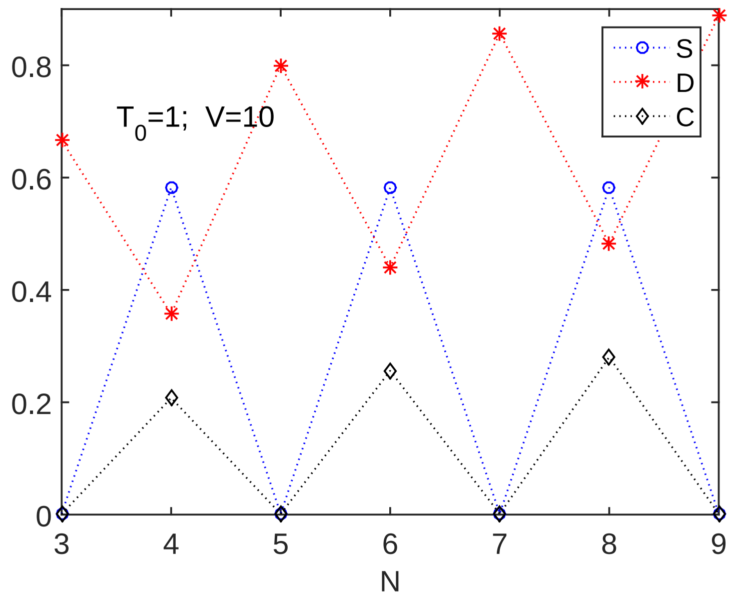

Figure 1. Statistical quantifiers (entropy S, disequilibrium D, and complexity C versus fermion-number N) at temperature = 1 Kelvin and coupling constant $V = 10$. The even-odd staggering effect is plainly visible.

4. Results

4.1. A Staggering Example

As just promised, Figure 1 exhibits our odd-even effect. Statistical quantifiers (entropy S, disequilibrium D, and complexity C) are plotted versus the fermion-number N at a temperature = 1 Kelvin, with the coupling constant $V = 10$. The even-odd staggering effect is plainly visible.

4.2. Model's Level-Spectra

We pass now to illustrate the behavior of our model's low-lying energy levels. For didactic purposes, we shift the energy scale so that the ground-state (GS) energy always equals zero. The temperature will always equal 1 Kelvin in our graphs.

Consider now a case in which the number N of fermions is even, for example $N = 6$ in Figure 2. We plainly see that the energy of the GS and that of the first excited state (1es) always lie close together as the coupling constant (cc) V augments.

Contrary wise, look at a case with an odd fermion number $N = 7$ in Figure 3. Things look quite different now, since only the GS separates itself from the remaining low lying states.

The same even-odd GS-1es pattern reported above is repeated for the pairs $N = k, k+1$ in the next four graphs, for $k = 10, 16$.

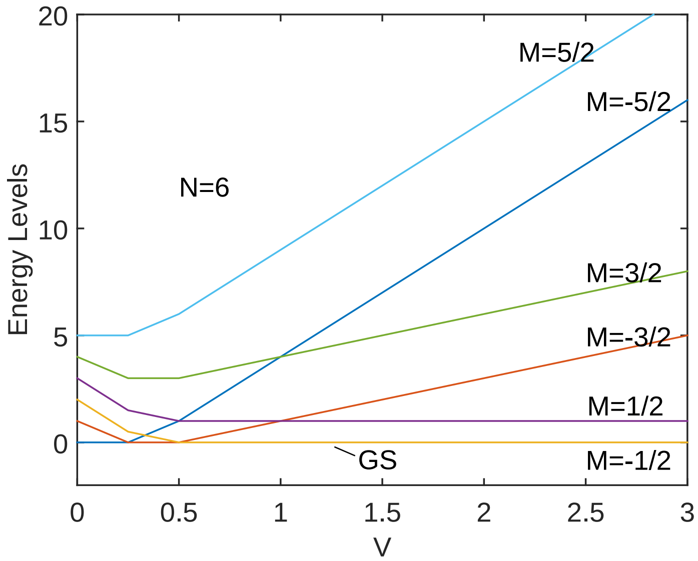

Figure 2. Level energies for the ground state (GS) and the first five excited states versus the coupling constant V of our fermion model. The number of fermions is $N = 6$. Energies are re-normalized so that the one for the ground state always equals zero. We note that the energy of the first excited (1ex) state (red line) is, for almost every $V-$value, very close to that of the GS. This fact results in two Boltzmann exponential factors of quite similar nature, i.e., similar probabilities. The remaining four excites states' energies (second to fifth) grow very rapidly with V and this distances them more and more from the almost constant energy pair [GS, 1ex]. This makes the respective probabilities of these four excited states grow progressively smaller. Probabilistically then, our scenario is dominated by the pair [GS, 1ex].

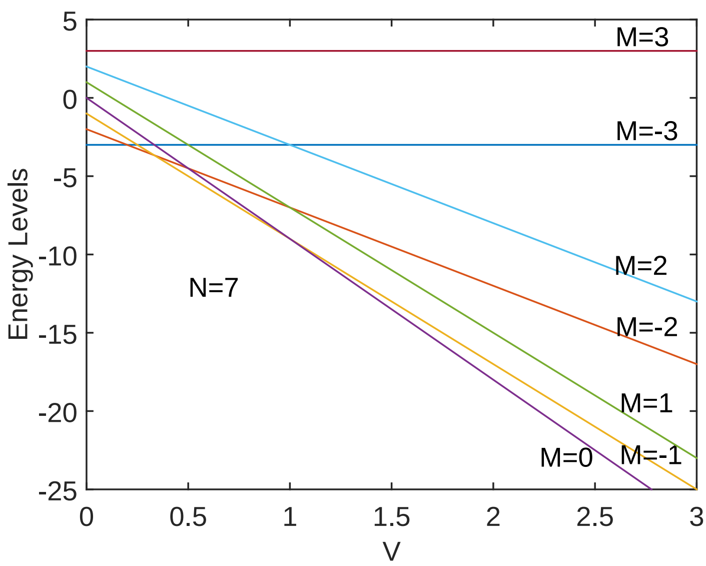

Figure 3. Model-energy levels versus coupling constant V for $N = 7$ fermions. Energies are re-normalized so that the one for the ground state equals zero always. Characterization of levels is like in Figure 2. It is clearly seen that, as V grows, the energetic distance between the ground state and all the excited states steadily augments.

4.3. Explanation

It is clear that the level-probabilities behave in the following manner

- For odd N, the largest probability in the partition function is by far that associated to the GS, E_0. Let us call it P_0, the energy of which is much lower than that of all the remaining states of energy $E_i >> E_0$. Thus, for all excited i, $P_i << P_0$.
- For even N, two different probabilities (those for the GS and for the 1st excited state) become appreciably larger than the ones for the rest of the energy levels. Thus, the entropy augments, as compared to that of the N-odd instance, and D consequently diminishes in the same fashion.
- Statistical odd-even staggering arises then because the entropy, for a given even N, is larger than that for its two neighbors $N-1$ and $N+1$.
- Odd-even staggering emerges thus as a spectral feature. In other words, it is a consequence of the Hamiltonian's nature. This nature is that of forward-scattering between the model's fermions [9]. Kramer's degeneracy is probably at play [25]. This is our main result.

5. Conclusions

We have shown that statistical odd-even staggering can be understood on the basis of the behavior of the low lying energy levels of our finite fermions model.

In other words, we showed that odd-even staggering (in our fermion model) is just the necessary consequence of spectral differences between odd or even systems.

These differences are then attributable to the pertinent Hamiltonian that describes forward scattering. Given the simplicity of the fermion–fermion interaction, our findings suggest that the observed odd-even differences are intrinsic, essential features of the fermionic nature.

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