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# Structure Evolution and Shape Phase Transitions in Odd-Mass Nuclei

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**Abstract.** The influence of the unpaired nucleon on the location and nature of phase transitions in odd-mass nuclei is an intersting issue. To study this, one needs to find adequate definition/choice of the control and order parameters, empirical signatures of the phase transition, and possible candidates for critical point nuclei. We present the evolution of the level structures determined by unique parity orbitals in odd-mass nuclei between Zn and Am, by correlations between excitation energies and ratios of such energies in both odd-mass nuclei and their even-even core nuclei. Clear evidence for a critical phase transition between the decoupling and strong coupling limits is found for nuclei in the mass 160 region around neutron number 90, which is closely correlated with the known critical shape phase transition in their even-even core nuclei from vibrator to rotor (the X(5) critical point). This abrupt change of structure is corroborated by a corresponding non-monotonic behavior of the differential variation of the two-neutron separation energy.

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## 1 Introduction

Quantum phase transitions in atomic nuclei are abrupt changes in the properties of the ground state due to competition between differemt shapes (shape phase transitions – SPT). Nuclear properties change when the number of nucleons changes, the critical (shape) phase transitions being rather rapid, when only several neutrons are added. Therefore, the number of neutrons, $N$, is a natural *control parameter* of the nuclear shape phase transitions. On the other hand, since $N$ does not vary continuously, the discountinuities at the phase transition point are smoothed out. Thus, although the quantum phase transitions in nuclei were theoretically discussed more than 30 years ago [1–3], they were experimentally recognized only much later [4, 5], by using as a control parameter an empirical structure property which has an almost continuous variation, such as the energy of the first excited $2^+$, $E(2^+)$ of the even-even nuclei. Many nuclear properties, when represented as a function of $E(2^+)$, show typical phase transition discontinuities at a certain critical value $E_c(2_1^+)$ [4]. SPT were extensively studied, both experimentally and theoretically, in the even-even nuclei; from theoretical point of view, Iachello introduced classes of symmetries as critical point solutions in addition to the three IBM dynamical symmetries [6], such as $X(5)$, $E(5)$ [7, 8]. Experimental studies also evidenced nuclei with properties close to those predicted by a critical point symmetry (e.g., for the X(5) symmetry, [9–11]).

SPT in odd-mass nuclei are much less studied in comparison with the even-even ones, the main reason being the large diversity of the low-energy excitations (determined by the shell model orbitals spanned by the unpaired nucleon), which makes it impossible to follow the evolution of the same quantity in many nuclei. In this work we propose a way of circumventing this problem, by presenting the evolution of the excited level structures in which the unpaired nucleon occupies an intruder (or unique parity) orbital. It is a very interesting issue to determine how the unpaired fermion influences on the nature and the location of the phase transition.

## 2 Odd-Mass Nuclei – Empirical Correlations

To study the phase transitions in the odd-mass nuclei one has, first, to identify structure observables that can be used as control and order parameters, respectively. Then, one can reveal the signatures of the quantum phase transitions, and possible critical point nuclei.

Our empirical study relies on the known experimental level structures stemming from the *intruder*, or *unique parity orbitals* (UPO). These structures are known to have extremely pure wave functions (high $j$-purity) because they do not mix with other orbitals. This leads to nearly dentical effects for any UPO, therefore one can use the same method (e.g., correlations between certain level struscture observables) to investigate many nuclei, actually, to cover consistent regions of the nuclear map.

We have investigated level structures based on the three most investigated UPO's, namely $1g_{9/2}$, $1h_{11/2}$, and $1i_{13/2}$. We found useful experimental data in ENSDF [12] for about 500 nuclei with $Z$ between 30 (Zn) and 95 (Am). The experimental data that we experimentally followed were excitation energies of states in the so-called *favored* (states of spin $j,\ j+2,\ j+4,\ ...$) and *unfavored* (spin $j+1,\ ,j+3,\ ...$) sequences, where $j$ is the spin of the UPO (e.g., 9/2 for $g_{9/2}$). A nucleus was saved in our database if at least the excitation energies $E^*(I)$ of the states of spin $j,\ j+2$ and $j+4$ were known, to which $E^*(j+1)$ was added, when known. Excitation energies relative to those of the state of spin $j$ were then defined: $E(I) = E^*(I) - E^*(j)$, with $I = j+2,\ j+4$ and $j+1$, and also ratios such as $R_{j+4/j+2} = E(j+4)/E(j+2)$ (similar to $R_{4/2} = E(4_1^+)/E(2_1^+)$ in the even-even nuclei), and $R^s_j = [E(j+2) - E(j+1)]/E(j+2)$, the latter, related to the energy difference between the favored and unfavored sequences being referred to as *signature splitting index*.

A suitable general theoretical framework to discuss the structure of odd-mass nuclei is the Particle-plus-Rotor Model(PRM) [13]. For low excitation energies of the UPO structures that we study, we consider the simple case of one nucleon moving in the potential of a deformed core with axial symmetry. Within this model there are three limit coupling schemes (for details, see [14, 15]), depending on the relative importance of the three main terms of the Hamiltonian: intrinsic (single-particle) motion, rotation of the inert core, and the Coriolis interaction. In short, these three coupling schemes, largely recognized in real nuclei, have the following characteristics:

(i) The **Weak Coupling**: it occurs for small deformations, up to $\beta_2 \approx 0.14$ (roughly corresponding to $R_{4/2}$ in the core nuclei between about 2.0 and 2.2. Charactertic of this coupling scheme is that the favored sequence of spins $j,\ j+2,\ j+4,$ ... has spacings similar to those of the g.s.b. $0^+,\ 2^+,\ 4^+,$ ... of the even-even core nucleus.

(ii) The **Strong Coupling**: occurs when the Coriolis interaction matrix elements are small compared to the s.p. energy splittings. This takes places for:

  (a) large deformations, $\beta_2$ above $\sim 0.24$ (or $R_{4/2} \gtrsim 3.0$);

  (b) small Coriolis matrix elements: for the large-$j$ UPO, this happens when the odd particle occupies a *high*-$\Omega$ orbital.

  In this coupling scheme the favored and unfavored sequences merge into a single $\Delta I = 1$ *rotational band.*

(iii) **Decoupling**: when the Coriolis interaction is strong and cannot be neglected. For the large-$j$ UPO this takes place when the odd particle is in a *low*-$\Omega$ orbital. This coupling limit appears for intermediate deformations, $\beta_2$ from about 0.14 to about 0.23 ($R_{4/2}$ roughly between 2.2 and 2.7). It is characterized by a favored sequence having spacings similar to those of the g.s.b. of the core nucleus, and the unfavored sequence lying at energies higher than those of the favored one..

In the *strong coupling* limit $R_{j+4/j+2} = (4j+10)/(2j+3)$ which is about 2.29 for all three cases considered by us, and the signature splitting index is $R^s_j \approx 0.54$ in the same cases.

Because the ratios $R_{4/2}$ in the even-even nuclei directly indicate the degree of collectivity (precollective nuclei for $R_{4/2} < 2.0$, and collective nuclei for $R_{4/2}$ between 2.0 and 3.33), we present first, in Figure 1, the correlation between the ratio $R_{j+4/j+2}$ in our $\sim$ 500 odd-mass nuclei and the $R_{4/2}$ ratio in their even-even cores. In this figure, we distinguish between nuclei with the unpaired nucleon of the *particle* type (filled symbols) and *hole* type (empty symbols),

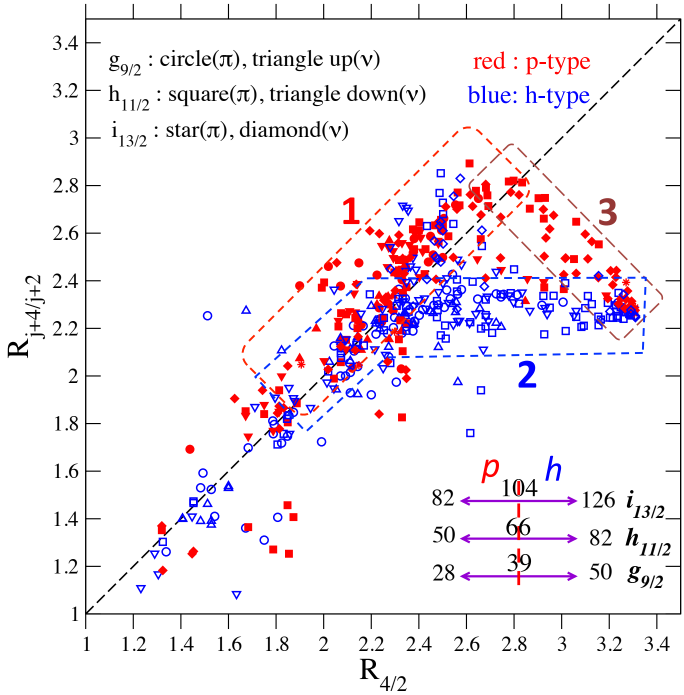


Figure 1. (color online) Correlation between the energy ratios $R_{j+4/j+2}$ of UPO favored sequences and $R_{4/2}$ of the even-even cores. The dashed line indicates equality of the two quantities. The symbols disclose both the UPO and the type (proton or neutron, particle or hole type) of the odd particle. The regions (boxes) marked by numbers are discussed in text.

when the unpaired nucleon number is below or above the middle of the major shell, respectivelly (as explained in the lower right shell diagram). The collective nuclei (that is, those with $R_{4/2} \gtrsim 2.0$) show a triangle-like structure. One remarks that, with few exceptions, the nuclei with particle-type unpaired nucleon occupy the upper two sides of this triangle, while those with hole-type nucleon lie on the lower side. For the sake of the discussion below, we divide the triangle pattern in three regions (the boxes marked 1, 2, and 3 in the figure). The evolution within regions 1 and 2 can be generally understood in terms of the PRM discussed above. Region 1 refers to the particle-like nuclei: around $R_{4/2} \sim 2.0$ (small deformations) they realize the *weak coupling*, then, with increasing deformation, up to $R_{4/2} \approx 2.7$, the nuclei realize the *decoupling* (case (iii), odd-particle in *low*-$\Omega$ orbitals from the lower half of the major shell). Region 2 refers to the evolution of the hole-type nuclei: *weak coupling* at low deformations ($R_{4/2} \leq 2.2$), followed by *strong coupling*, either because the nucleon occupies now *high*-$\Omega$ orbitals (from the higher half of the major shell), or the deformation is high ($R_{4/2} \approx 3.30$).

The few cases of hole-type nuclei mixed up with the particle-type ones in the decoupling part of region 1 are due to nuclei known to have *oblate* shapes (they correspond mainly to the Au and Hg nuclei with holes in the proton $h_{11/2}$ orbital and neutron $i_{13/2}$ orbital, respectively). If the deformation is oblate, then, for the hole-type nuclei the situation is reversed with respect to that of the particle-type described above: now the unpaired nucleon occupies *low*-$\Omega$ states, which leads to the decoupling situation.

Region 3 comprises nuclei that realize a direct transition between the decoupling and strong coupling limits, at large deformations ($R_{4/2}$ around 3.0). This special transition will be examined in detail in the following section.

## 3 Critical Phase Transition in the Odd-Mass Nuclei

The region marked 3 in Figure 1 shows a very interesting transition when the evolution along isotopic chains of nuclei is considered. The nuclei in this region correspond to $\pi h_{11/2}$ structures in the La, Pr and Pm isotopes around $N = 70$, and $\nu i_{13/2}$ structures in Sm, Gd, Dy Er, Yb, Hf and W isotopes around $N = 90$. We analize in detail the case of the $\nu i_{13/2}$ structures for which experimental data were found for a large number of nuclei (about 50).

Figure 2 displays different correlations for these nuclei, in which the number of neutrons $N$ spans values from 83 to about 109. One remarks that these experimental data form rather compact trajectories. Panel (a) shows the correlation between $R_{j+4/j+2}$ in odd-mass nuclei and $R_{4/2}$ in their even-even nuclei. With increasing $N$ (starting from $N \sim 83$) and decreasing $E(2^+)$, $E(j+2)$ decreases up to a value of about 200 keV, thereafter increasing very rapidly although $E(2^+)$ continues to decrease. The minimum value $E_c(j+2) \approx 200$ keV is reached at the value $E_c(2^+) \approx 140$ keV, for nuclei with $N$ values of about 90. The $E_c(2^+)$ is known as the *critical point* of the shape phase transition from nuclei with an anharmonic behavior to deformed nuclei, with a rotor behavior [4], this point being associated with the X(5) critical symmetry [7]. Panel (b) presents the evolution of the favored bands, in terms of the correlation between $E(j+4)$ and $E(j+2)$ in the odd-A nuclei, a plot similar to $E(4^+)$ versus $E(2^+)$ in the even-even cores. The $E_c(j+2) \approx 200$ keV value appears as a *turning point*, which separates nuclei that evolve along two branches: on the upper branch, with increasing $N$, both $E(j+4)$ and $E(j+2)$ decrease (the favored band compresses), along a line of slope about 1.8 (decoupling); after the turning point, they follow a trajectory which goes assimptotically towards a line of slope 2.25 (strong coupling). Around $E_c(j+2)$ the evolution from decoupling to strong coupling is rather fast - it takes place within just a few isotopes. Actually, at the turning point the derivative of $E(j+4)$ with respect to $E(j+2)$ is discontinuous having $E_c(j+2) \approx 200$ keV as a vertical assymptote: with increasing $N$ it varies from a constant value of about 1.8 to $+\infty$ at

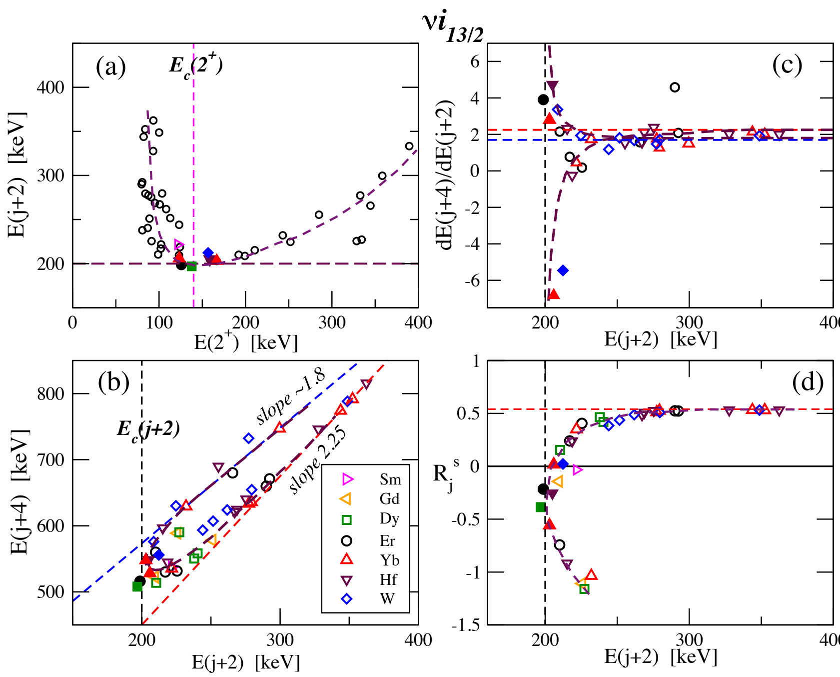


Figure 2. (color online) Correlations illustrating the critical phase transition between the decoupling and strong coupling limits of $\nu i_{13/2}$ structures (contour nr. 3 in Figures 1 and 2). (a) Rapid change of $E(j+2)$ evolution around the critical value $E_c(2_1^+) \approx 140$ keV corresponding to the critical point of the core nuclei; (b) "Turning point" behavior in the $E(j+4)$ versus $E(j+2)$ graph. (c) Derivative of the trajectory from graph (b); (d) Evolution of the signature splitting index $R_j^s$. The dashed lines in (a),(b) and (d) are drawn by hand through the data points, while the long-dashed line in (c) is the derivative of the corresponding continuous curve from (b). Filled symbols mark the nuclei closest to the critical point (see text).

$E_c(j+2) \approx 200$ keV, then from $-\infty$ towards a constant value of 2.25. This discontinuous behavior is similar to that of the quantity $dE(4^+)/dE(2^+)$ in the even-even nuclei, which has the features of order parameter of a first order critical phase transition [4]. Therefore, $E_c(j+2)$ is a genuine critical point of the transition between the decoupling and strong coupling limits. Graph (d) finally shows the evolution of the signature splitting index $R_j^s$ with $E(j+2)$ which varies from large negative values (decopupling) to a value of +0.54 (strong coupling), again having $E_c(j+2)$ as a turning point. One can see that close to the critical point most of the nuclei have $R_j^s \approx 0$, that is, the states of the favored sequence are alomost degenerated in energy with those of the unfavored one. In all graphs (a) to (d) the nuclei closest to the critical point of the transition (the turning point) were represented by filled symbols. These nuclei are proposed as

Table 1. Odd-mass nuclei close to the critical point $E_c(j+2) \approx 200$ keV of the transition from decoupling to strong coupling, as deduced from the behavior of the $\nu i_{13/2}$ structures. See additional explanations in text.

| Nucleus | Core nucleus | $N$(core) | X(5) | $R_j^s \approx 0$ |
|---|---|---|---|---|
| $^{153}$Sm$^{62}$ | $^{152}$Sm | 90 | X | X |
| $^{155}$Gd$^{64}$ | $^{154}$Gd | 90 | X | (X) |
| $^{157}$Dy$^{66}$ | $^{156}$Dy | 90 | X | (X) |
| $^{161}$Er$^{68}$ | $^{160}$Er | 92 | (X) | |
| $^{163}$Yb$^{70}$ | $^{162}$Yb | 92 | (X) | |
| $^{165}$Yb$^{70}$ | $^{164}$Yb | 94 | | X |
| $^{167}$Hf$^{72}$ | $^{166}$Hf | 94 | (X) | |
| $^{171}$W$^{74}$ | $^{170}$W | 96 | (X) | X |

best candidates for critical point nuclei, and are summarized in Table I. The fifth column shows the extent to which the core nucleus is considered to realize the X(5) critical point ("X" and "(X)" denote nuclei that fulfill reasonably well, or only to a certain extent, the X(5) predictions for the g.s.b. excitation energies and $B(E2)$ values, respectively), according to [9–11]. The sixth column shows how well the condition $R_j^s = 0$ is fulfilled ("X" and "(X)" means that for the first states of the favored and unfavored band the energy degeneracy is fulfilled within a few keV, and several tens of keV, respectively) [12].

From the above analysis it results that the critical phase transition found in these nuclei is closely related to that encountered in the even-even core nuclei around $N = 90 - 92$ (with the X(5) critical point of the transition between anharmonic vibrators and rotors). The best candidates of nuclei with critical point features are those closest to the turning point in Figure 2, graphs (b) and (c), another signature of the critical point probably being the energy degeneracy of their favored and unfavored sequences.

The proton-odd nuclei from La ($Z = 57$) to Tb ($Z = 65$), where $\pi h_{11/2}$ structures are known [12] could also form a similar region of critical phase transition around $N = 90$. However, for these nuclei the UPO structures are known only for nuclei with $N$ up to 90 or 92, therefore one could not really highlight a critical (turning) point behavior.

On the other hand, another region where one encounters a transition with similar features is that of the La, Pr and Pm nuclei (with $\pi h_{11/2}$ sequences) [16]. For these nuclei the critical energy is $E_c(j+2) \approx 235$ keV and the turning points for the different isotopic chains approximately correspond to $^{125}$La, $^{127}$Pr or $^{129}$Pr, and $^{133}$Pm, having as cores $^{124}$Ba, $^{126,128}$Ce, and $^{132}$Nd, with $N = 68, 70$ and 72, respectively, all having yrast states energies close to the X(5) predictions [10].

## 4 Additional Evidence for Critical Phase Transitions in Odd-Mass Nuclei

Nuclear masses are known to clearly disclose the regions where important structural changes are taking place. We have examined the behavior of the two-neutron separation enegies $S_{2n}$ of the odd-mass nuclei considered in this work. To better display non-monotonic variations we have in fact taken the differential of this quantity $dS_{2n}(Z,N) = [S_{2n}(Z,N+2) - S_{2n}(Z,N)]/2$ calculated from values given in the mass tables [17]. Figure 3 displays the evolution of $dS_{2n}$ of nuclei with $Z$ between 54 and 74 and $N$ values between 72 and 114. The

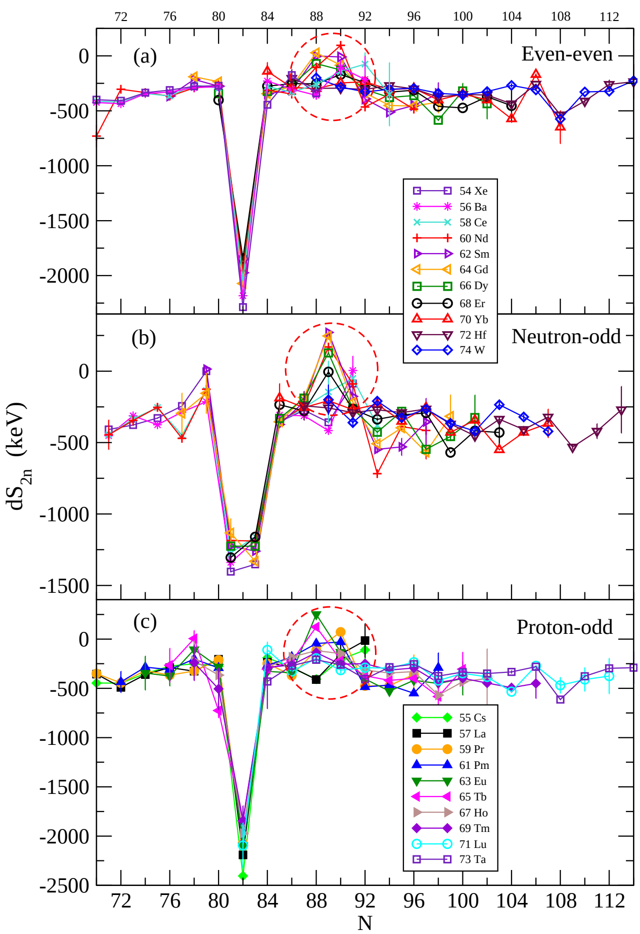


Figure 3. (color online) Differential variation of the two-neutron separation energy for nuclei discussed in this work.

major shell closure at $N = 82$ is marked by a big negative spike and another negative spike occurs at the known deformed shell closure at $N = 108$. Another drastic structural change appears as a positive irregularity at $N = 88 - 92$. For the even-even nuclei this was related to the critical shape phase transition that takes place around $N = 90$ (the X(5) critical point) [18]. For the odd-mass (both neutron-odd and proton-odd) nuclei, one observes similar irregularities, which correspond to the phase transitions discussed above. Actually, for the even-even nuclei it was shown that the differential variation of other observables (like $< r^2 >$, $E(2_1^+)$, $R_{4/2}$, and $B(E2, 2_1^+ \rightarrow 0_1^+)$) show a behavior similar to that of $dS_{2n}$ [19].

## 5 Conclusions

By studying the evolution of relative excitation energies and their ratios for states within the favored and unfavored sequences of structures based on unique parity orbitals, clear evidence of a critical phase transition in odd-A nuclei was obtained, correlated with that known to take place in their even-even core nuclei. It was found that $E(j + 2)$ can be successfully used as a control parameter, whereas $E(j+4)$ or rather, its derivative $dE(j+4)/d(E(j+2)$ are useful order parameters (similar to $E(2^+)$, $E(4^+)$, and $dE(4^+)/dE(2^+)$ in even-even nuclei). For the $\nu i_{13/2}$ structures of nuclei around $N = 90$ and $\pi h_{11/2}$ structures in nuclei around $N = 70$ this phase transition shows up as a rapid transition from the decoupling limit to the strong coupling limit, which is correlated with the shape phase transition between vibrator and rotor in the even-even nuclei from the same region. This rapid nuclear structure transition is corroborated by strong irregularities observed in the variation of the two-neutron separation energies. Details of structure evolutions in other nuclear regions shown in Figure 1 are given in Ref. [16].

It is interesting to extend the study of shape phase transitions in the odd-mass nuclei by considering other structure observables that can be used as control and order parameters, such as suggested by the study in Ref. [20]. It is also interesting to consider what other observables could be used in order to support/highlight the phase coexistence picture. The study may be extended by theoretical understanding of the empirical observations reported here in terms of structure models such as the Interacting Boson-Fermion Model [21] or the critical point symmetry model X(5/(2j+1)) [22].

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