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Nuclear Shell Model And Quantum Phase Transitions

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Abstract   The usual nuclear shell model defines nuclear properties through an effective mean-field plus a two-body interaction Hamiltonian in a finite orbital space. In this study we try to understand the correlation between the various parts of the shell model Hamiltonian and the nuclear observables and collectivity in nuclei. By varying specific groups of matrix elements we find signs of a phase transition in nuclei between a non-collective and a collective phase. In all cases studied the collective phase is attained when the single-particle transfer matrix elements are dominant in the shell model Hamiltonian, giving collective characteristics to nuclei.

Keywords   quantum phase transitions, nuclear shell model

INTRODUCTION

Nuclear models have long provided a fertile ground for studying phase transitions in mesoscopic quantum systems. Quantum phase transitions [1–6] occur when the special observables of a system, called order parameters, reveal structural, often geometrical, changes as a function of control quantities. The search of quantum phase transitions is performed by writing the Hamiltonian in this form

$$H = (1 - \lambda)H_1 + \lambda H_2.$$

By varying the control parameter λ, the system moves between the limiting symmetries H_1 and H_2 and one might find a critical value of the control parameter, λ_c, where a quantum phase transition is observed. The existence of the quantum phase transition and its order is confirmed using the Ehrenfest criterion [7], which involves the study of the derivatives of the ground state energy functional. If the first derivative with respect to λ is dicontinuous, then we have a first order quantum phase transition. If the second derivative is discontinuous, then the quantum phase transition is of second order. If no discontinuity is found, there is no quantum phase transition, only a crossover between the two phases.

In the framework of the shell model, pairing and collective effects are fully taken into account through the two-body interaction matrix elements. In the following, we explore the effects of specific components of the effective shell-model interactions on the properties of nuclear spectra, and identify the patterns related to the effects of certain parts of these interactions. In particular, we study the qualitative changes of nuclear observables similar to phase transitions which appear as a function of the interaction in the same shell-model

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framework. In this way we expect to better understand the relationship between the input effective Hamiltonian and the nuclear output. By changing the interaction matrix elements for a single nucleus, we can no longer reproduce the nuclear properties of this particular nucleus, however, it has been found that [8, 9] even a random (but keeping in force angular momentum and isospin symmetry) set of matrix elements in a finite orbital space results in the energy spectrum and properties of stationary states which carry certain analogies to realistic nuclei.

In the case of the sd shell model space we have only three single-particle levels, $2s_{1/2}, 1d_{5/2}, 1d_{3/2}$. The angular momentum and isospin conservation allow 63 matrix elements of the residual two-body interactions. Similarly, the two-body interaction in the pf shell, which is made up of the $1f_{7/2}, 2p_{3/2}, 1f_{5/2}, 2p_{1/2}$ single particle levels, has 195 non-zero matrix elements. In a recent study [10], where the pf orbital space was used, it was found that certain interaction matrix elements are responsible for the transition from a spherical shape to a deformed one. First of all, these were the matrix elements (pf matrix elements in that specific model) changing the occupation numbers of the subshells by one unit, i.e. the matrix elements $\langle j_k, j_l | V | j_m, j_n \rangle$ with $j_k = j_m$, or $j_k = j_n$, or $j_l = j_m$, or $j_l = j_n$. This drives the mixing of spherical orbitals in the process of deformation. A complementary version of a similar approach was applied in [11] in order to demonstrate that the incoherent parts of the residual interaction are essential for producing chaotic wave functions and resulting smooth level density.

QUANTUM PHASE TRANSITIONS

Borrowing the previous approach, we divide the set of interaction matrix elements into two parts. The part V_1 includes the "particle-hole" matrix elements which change the occupation number of the subshells by one unit (from now on "one unit change matrix elements"), whereas part V_2 includes the remaining matrix elements, which either don't change the occupation number of the sub shells ($j_k = j_m$ and $j_l = j_n$), or change it by two units ($j_k \neq j_m$ and $j_l \neq j_n$). By writing the Hamoltonian in the form

$$H = h + (1 - \lambda)V_1 + \lambda V_2 \quad (1)$$

where part h containing the single particle energies remains fixed and λ is the control parameter, we vary λ from 0 to 1 in steps of 0.1 and study phase transitional patterns in even-even, odd-odd and odd-A nuclei in the sd and pf shells. In the sd shell model space we have results for ^{24}Mg, ^{28}Si, which represent the even-even cases and $^{26-28}$Al, ^{30}P, which represent odd-odd and odd-A cases. We also chose the ^{52}Fe and ^{50}Mn nuclei, to represent an even-even and odd-odd case, respectively, in the pf shell. We have focused our interest mainly to the evolution, as a function of λ, of the energy states, reduced transition probabilities, quadrupole moments and wave function amplitudes of the ground state, though also higher spin states have been taken into consideration for odd-odd and odd-A nuclei. The results can be found in the figures which follow.

For even-even nuclei, the λ dependence of the low-energy levels presents a minimum at λ around 0.2-0.3 for all nuclei and for almost all values of nuclear spin. At the same time, the

energy ratio $R_{4/2}$ reaches a maximum, which is always close to a deformed value, just after, or at, the minimum in the energies of the yrast states. The ratio $E(J)/J(J+1)$ (effective inverse moment of inertia) is almost independent of J, from $\lambda = 0$ up to the value of λ where the energy ratio $R_{4/2}$ has its maximum value for each particular nucleus. The reduced transition probabilities are also sensitive to the phase transition, showing a maximum close to the point of the minimum energy of the yrast states, as seen in figures 1, 2 and 3.
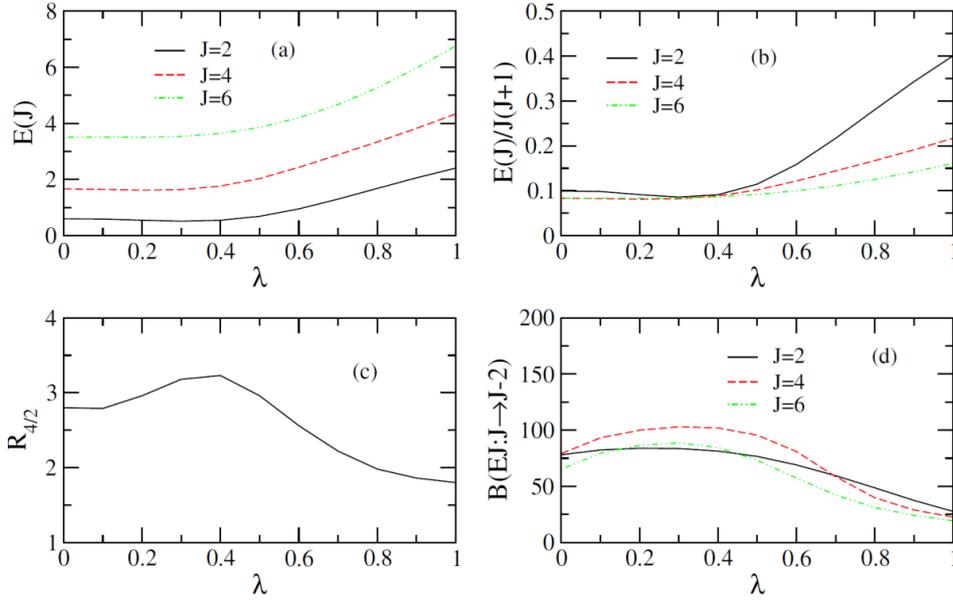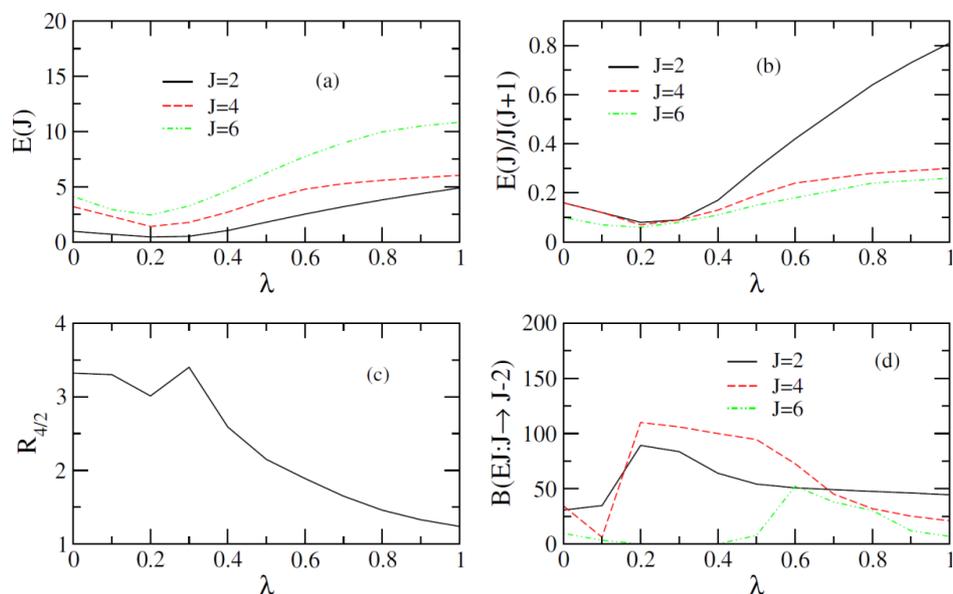

Fig. 1. (a) Yrast 2^+, 4^+, 6^+ energies, (b) ratios $E(J)/J(J+1)$ for J = 0, 2, 4, (c) ratios $R_{4/2}$, (d) electromagnetic transition rates as a function of λ for ^{24}Mg.

The ground state wave function also displays the signs of a quantum phase transition. The left panel of figure 4 shows the percentage of coupling of protons and neutrons to angular momenta $(J_n, J_p) = (0,0), (2,2), (3,3), (4,4), (6,6)$ of the ground state 0_1^+, as a function of λ. For even-even nuclei, up until the point of the quantum phase transition, the (2,2) coupled pairs are the strongest components of the ground state wave function, a behavior consistent with deformational characteristics. After the critical point, their amplitudes fall and the amplitudes of the (0,0) coupled pairs rise, becoming eventually the strongest components of the wave function, a typical feature of the vibrational limit.

While for even-even nuclei the λ dependence of the energies presents a minimum only for the first few yrast low-energy levels, for odd-odd or odd-even nuclei the minimum persists up to high energy values, showing that the unpaired nucleon greatly affects the results of this study. For yrast states, figure 5, there is a clear minimum of the level energy for all nuclei studied. In figure 6 the behavior of the reduced transition probabilities B(E2; $2_1^+ \to 0_1^+$), B(E2; $2_1^+ \to 1_1^+$), B(E2; $6_1^+ \to 4_1^+$) and quadrupole moments of ^{26,28}Al is presented. In all cases (even for those not appearing in figure 6) there is a maximum of the transition rate in the region where the signal of a phase transition appears in energies. The quadrupole

moment, despite the fact that it changes abruptly due to the details of the interaction, it also shows signs of a quantum phase transition. In all cases, the quadrupole moment takes its maximum value at those values of λ for which the quantum phase transition takes place, dropping to smaller values for λ closer to 1.
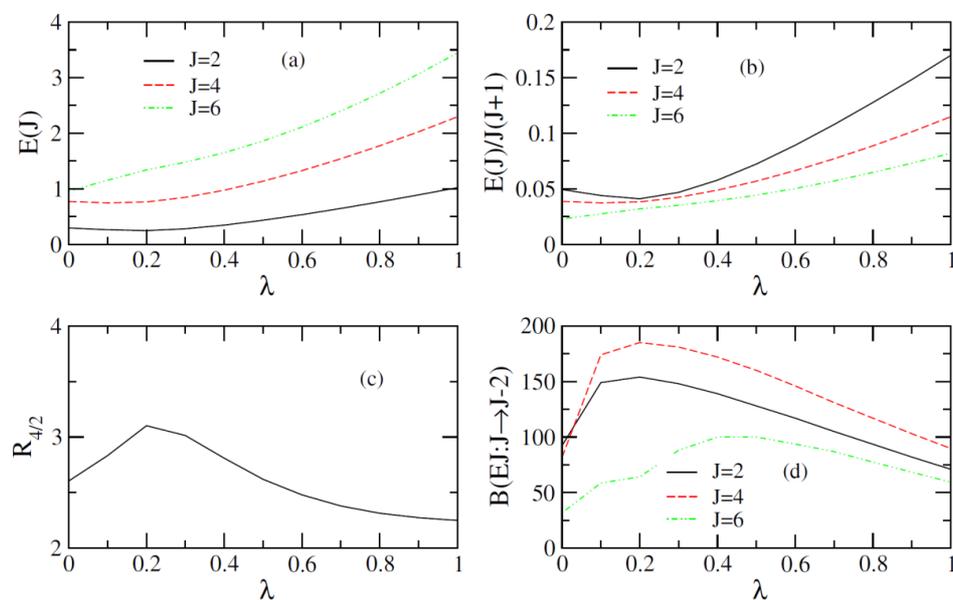

Fig. 2. (a) Yrast 2^+, 4^+, 6^+ energies, (b) ratios $E(J)/J(J+1)$ for $J = 0, 2, 4$, (c) ratios $R_{4/2}$, (d) electromagnetic transition rates as a function of λ for ^{28}Si.

Fig. 3. (a) Yrast 2^+, 4^+, 6^+ energies, (b) ratios $E(J)/J(J+1)$ for $J = 0, 2, 4$, (c) ratios $R_{4/2}$, (d) electromagnetic transition rates as a function of λ for ^{52}Fe.
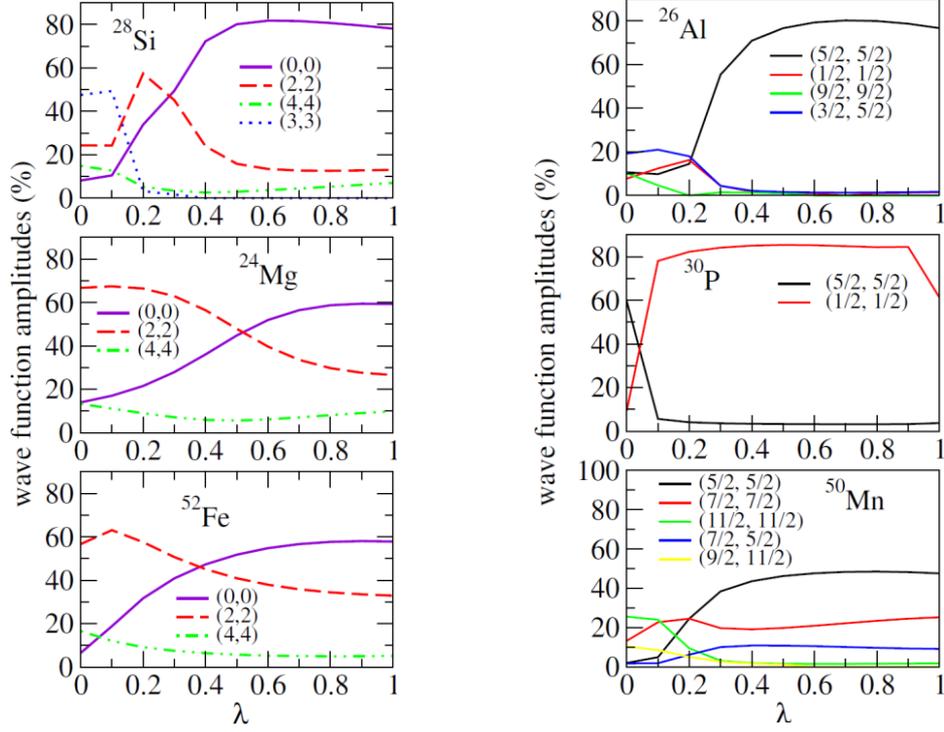
Fig. 4. Left panel: Amplitudes of the wave function 0^+_1 expanded in terms of proton and neutron angular momenta as a function of λ for ^{28}Si, ^{24}Mg, and ^{52}Fe, Right panel: Amplitudes of the wave function 1^+_1 expanded in terms of proton and neutron angular momenta as a function of λ for ^{26}Al, ^{30}P, and ^{50}Mn.

The proton and neutron spin decomposition of the wave functions of different stationary states also presents signs of a quantum phase transition. In figure 4, right panel, we show the decomposition of the wave function of the 1^+_1 state that serves as the ground state for some values of λ in all studied nuclei, but only those components which have an amplitude over 10%. First, there is an abrupt change of the spin decomposition at the transitional point. Second, before the transitional point, there is a strong mixing of the wave function components, while after the transitional point there are one or two dominant components, with the rest falling to a minuscule contribution.

All these results suggest that there is a quantum phase transition taking place as the values of the V_1 matrix elements increase. As stated in the introduction, in order to be sure that a quantum phase transition is present, the Ehrenfest criterion must be applied, which will also provide the order of the transition. In Figure 7 we look for discontinuities at the first and second derivatives of the ground state energies of ^{26}Al and ^{27}Al. The upper panel of Figure 7 shows the ground state energies of ^{26}Al and ^{27}Al as a function of λ, while the middle and lower panels show the first and second derivative of the ground state energies, respectively. The ground state energy appears to be a smooth function of λ, however, sudden jumps appear at the first derivative of the ground state energy, which correspond to steep minima at the second derivative. These minima reflect the proton and neutron spin decomposition of the wave function, as well as the single – particle orbital occupancies of the ground state. After each spike of the second derivative, the ground state structure changes from a mixed to a pure configuration, reflected in the rising of a single-particle orbital occupation and the rising of a

less mixed proton and neutron coupling configuration. From the study of the derivatives of the ground state wave function we understand that this is a second order phase transition.
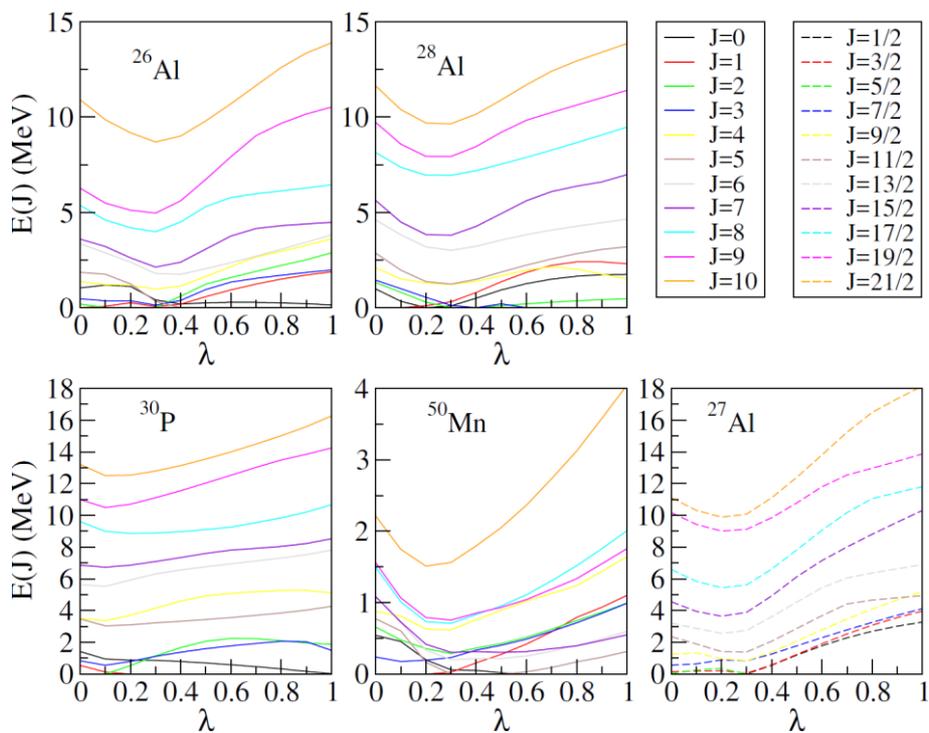

Fig. 5. Yrast energies of J = 0 - 10 in ^{26,28}Al, ^{30}P, and ^{50}Mn and J = 1/2 - 21/2 in ^{27}Al, as a function λ.
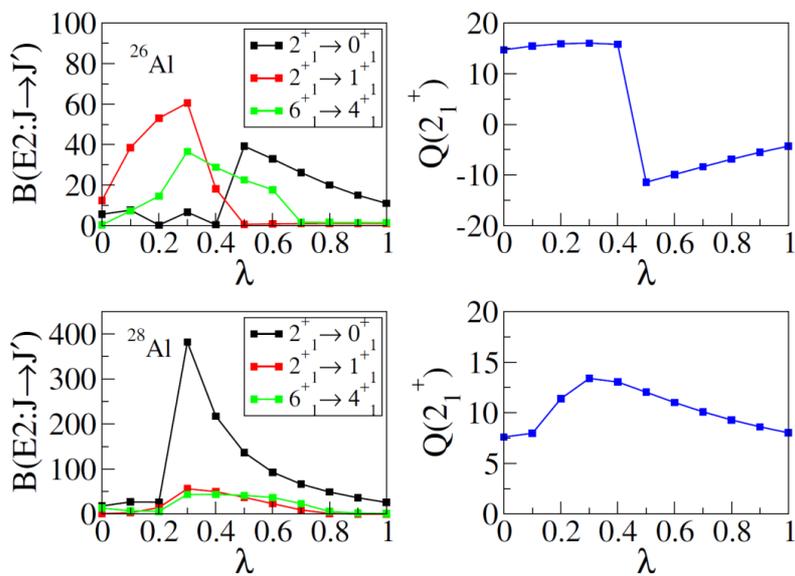

Fig. 6. Reduced quadrupole transition probabilities and quadrupole moments as a function λ for ^{26,28}Al.
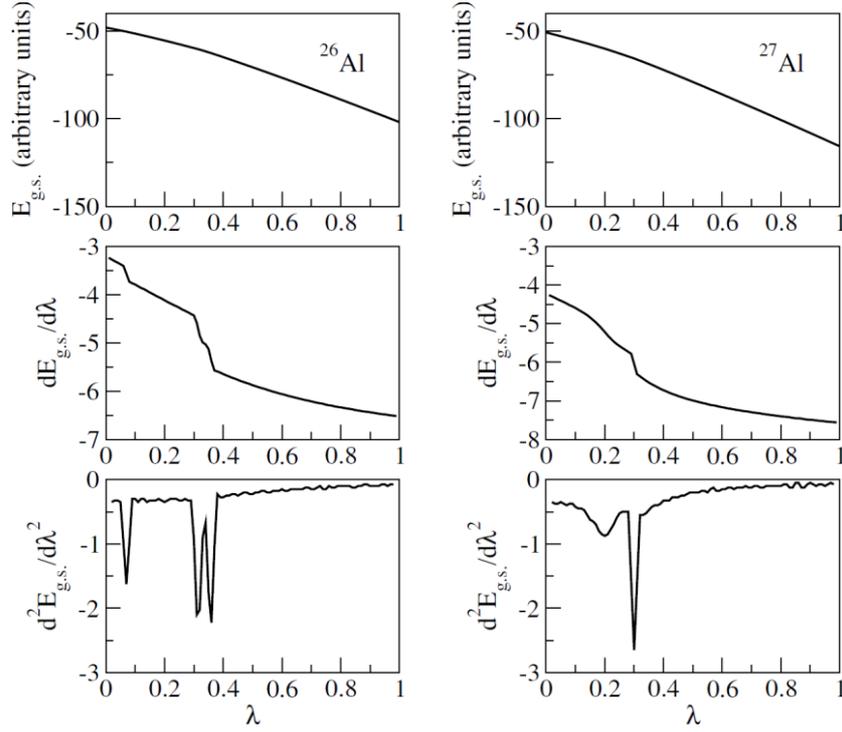
Fig. 6. The ground state energy and its first and second derivatifves for ^{26,27}Al as a function of λ.

CONCLUSIONS

Summarizing, we studied the evolution of some nuclear observables when varying the values of specific matrix elements of the shell model Hamiltonian. We divided the two-body shell model interaction Hamiltonian into two parts, one containing the "one-unit change" interaction matrix elements and the other containing the rest two-body matrix elements. The results of the energy levels, multipole transition probabilities, the wave function decomposition in proton and neutron spin components, and the quadrupole moments for all the selected nuclei of the sd and pf shell, reveal the same coherent picture. At some critical value of λ, all nuclei undergo a transition from a mixed and collectively deformed phase to a phase close to the spherical shape for larger values of λ. The "one-unit change" matrix elements are responsible for inducing deformational characteristics on nuclei and it appears that they act more strongly on unpaired fermions. Also, the study of the derivatives of the ground state wave function suggests that this is a second order phase transition.

There is a principal difference between the nuclear models, mainly algebraic, where the quantum phase transitions are studied, and the framework we used to induce a quantum phase transition. In the first case, a system is moving between two well defined symmetries, while in our case the two groups of matrix elements are not directly related to any explicit symmetry. The results, though, show clear signs of a qualitative change in all studied observables of nuclei, as a function of λ. There is no unique critical value of λ where this

qualitative change takes place, as the interaction affects different nuclei differently. However we clearly see a coherent behavior of various observables in different nuclei.

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