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Shell evolution and emerging paradigm changes

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Abstract. The shell structure conceived by Mayer and Jensen in 1949 has been shown to be quite appropriate for stable and near-stable nuclei, but substantial deviations from it have also been observed more recently for exotic nuclei with notable neutron excess. Such changes of the basic picture of the nuclear shell structure, called the shell evolution, seem to be the subject studied most extensively and most elaborately by RI beam experiments worldwide. An overview of the shell evolution is presented in this talk, from both theoretical and experimental perspectives. The shell structure is shown to be varied, for instance, from the one presented by Mayer and Jensen, by particular types of the monopole components of the effective nucleon-nucleon interaction in nuclei. Among various contributions, the importance of the tensor force is illuminated here, with an outstanding example: the emergence of new neutron magic number 34 in neutron-rich Ca isotopes. The mechanism of the shell evolution produces significant impacts also on the nuclear shapes. Type II shell evolution shifts the excitation energies of intruder deformed bands, for instance, in some Ni isotopes. In other more general cases, the monopole interaction is shown to produce unexpected crucial effects on the patters of rotational bands of heavy deformed nuclei. In fact, the shape of the ellipsoidal deformation is investigated by large-scale shell model calculations, which is nothing but the Monte Carlo Shell Model. The unique role of the monopole component of the tensor force is clarified: the interplay between this monopole interaction and the quadrupole interaction provides us with various patterns of triaxial shapes for many nuclei, such as ^{166}Er, one of the traditional prolate deformed heavy nuclei. Thus, the prolate preponderance hypothesis by Aage Bohr is investigated for its microscopic validity. Some of the nuclear paradigms are changing now in this way, due to emerging aspects of nuclear-force effects.

1. Introduction

The shell evolution is one of the major developments promoted by the Rare-Isotope physics. I first present an introduction of the shell evolution and a current landscape of magic numbers and shell structure, by quickly overviewing selected items [1]. I then move on to heavy nuclei, such as rare-earth nuclei, where strong deformation dominates the structure of low-lying states. It is clear that the shell structure is not so visible due to the deformation, but the same interactions that bring about the shell evolution are still in action. In fact, these interactions are shown to produce unexpected effects on nuclear shapes. Thus, the understanding of nuclear structure has been and is being changed even at the very underlying levels, such as the shell structure and the nuclear shapes. Here, I try to sketch them.

2. Shell evolution

The shell structure and magic numbers conceived by Mayer [2] and Jensen [3] have guided us in the study of nuclear structure. The shell structure obtained from the harmonic oscillator potential + spin-orbit splitting produces a reasonable framework also for modern nuclear structure calculations. However, some changes are needed. The Mayer-Jensen scheme is based on the short-range attraction of nuclear forces and the density saturation inside the nucleus [4]. The predicted shell structure looked quite adequate, indeed with great successes. Just minor modifications of single-particle energies (SPE) were needed for individual cases. However, for neutron-rich exotic nuclei, the situation appeared to be different: there are certain effects due to parts of nuclear forces not fully incorporated in the Mayer-Jensen scheme [4], up to inversions of singe-particle orbits from the ordering given by the Mayer-Jensen scheme.

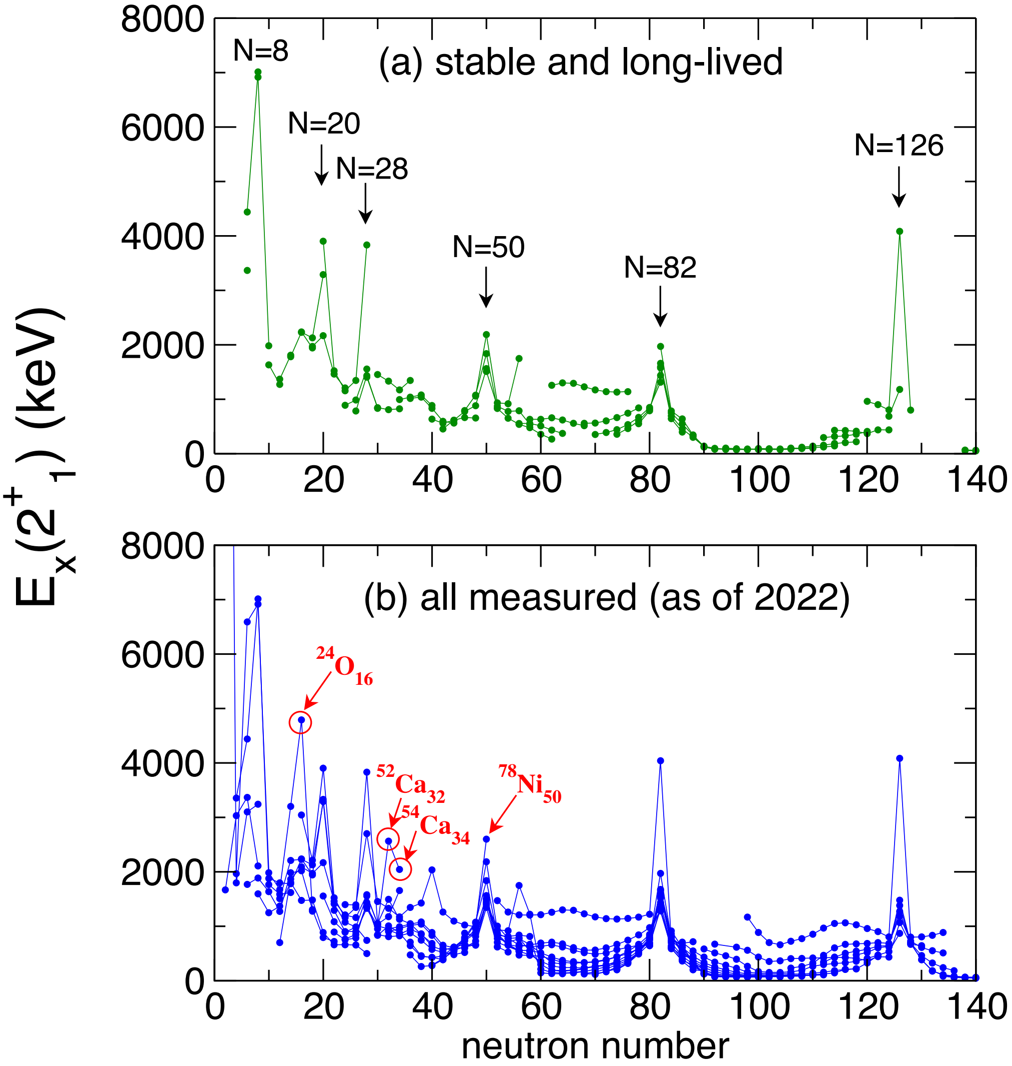

Figure 1. Systematics of the first 2^+ excitation energies of even-even nuclei as a function of the neutron number (N). **a** For those of all stable and long-lived nuclei. **b** All measured as of the year 2022. In **a**, the spikes correspond to magic numbers, N=8, 20, 28, ... In **b**, new magic numbers are shown by spikes somewhat lower, and are indicated by the corresponding nuclei in red. Figure courtesy of Y. Utsuno.

It is well known that the lowest 2^+ level energies are a good indicator of the magic gaps. Figure 1**a** displays these values of stable and long-lived nuclei, where all conventional magic numbers from N=8 to N=126 are identified.

Figure 1**b** depicts more points. Besides the spikes already seen in Fig. 1**a**, new peaks are found for N=16, 32, 34 in addition to N=50. I did not put the indicator for the 2 MeV peak of N=40 (harmonic oscillator magic number at ^{68}Ni), only because it may not be new. It is of interest that new magic numbers, including N=50, yield somewhat lower 2^+_1 level energies as compared to old magic numbers. Namely, the old magic numbers, excluding N=50, provide the 2^+ level energies around 4 MeV or higher. The new magic numbers are between 2 and 3 MeV except for N=16. The higher value at N=16 may be an exception due to a possible mass-number (A) dependence or something else. It is of interest to understand what physics can be behind this "magic 2^+ hierarchy", although it is often simply stated, also in this conference, that we can find many magic numbers (period !).

We also notice that the observation of new magic numbers is stopped at ^{78}Ni. This is, of course, due to the deformation in heavier nuclei, and I will come back to this topic.

We now turn to theoretical discussions as to why such new magic numbers appear, or more generally, how the shell structure changes as Z or N changes. For this purpose, we introduce a monopole interaction, that is an average of any two-body interaction. A short description of the monopole interaction can be found in [4], while more details are provided in [1] including some earlier works such as [5]. The matrix element of the monopole interaction is given by,

$$V^{mono}(j,j') = \frac{\Sigma_{(m,m')} \langle j,m\,;\,j',m'|\hat{V}|j,m\,;\,j',m'\rangle}{\Sigma_{(m,m')}\,1}, \tag{1}$$

where $\hat{V}$ is the interaction of interest, j and j' refer to single-particle orbits, m and m' denote their magnetic substates. This quantity does not depend on the angular momentum coupled by $\vec{j}$ and $\vec{j'}$, because the angular dependences are averaged out. It changes SPE: for instance, the difference of a proton SPE is expressed as

$$\Delta\epsilon^p_j = \Sigma_{j'}\, V^{mono}_{pp}(j,j')\,\Delta n^p_{j'} + \Sigma_{j'}\, \tilde{V}^{mono}_{pn}(j,\,j')\;\Delta n^n_{j'}\,, \tag{2}$$

where $\Delta n^p_{j'}$ ($\Delta n^n_{j'}$) stands for the difference of the expectation value of the occupation number of individual orbit $n^p_{j'}$ ($n^n_{j'}$), between two states (e.g. ground states of two isotopes). We have a similar equation for the neutron SPE.

While any interaction has its monopole interaction, the monopole interaction of the tensor and central forces are of particular relevance. The effect of the tensor force on the SPE changes its sign between the case of j=l+1/2 and j'=l'+1/2 and the case of j=l+1/2 and j'=l'-1/2. The former is always repulsive, whereas the latter attractive. This feature is visualized in Fig. 2 (Left).

The central force generates an attractive monopole interaction. Because nuclear forces are stronger in the isospin T=0 channel than in the T=1 channel, we restrict ourselves to monopole (interaction) effects between a proton and a neutron. Both the tensor and central forces yield monopole interactions of larger magnitudes between (i) spin-orbit partners like $1f_{7/2}$ and $1f_{5/2}$, and (ii) two orbits with the largest orbital angular momenta within a harmonic oscillator shell like $1f_{7/2,5/2}$ and $1g_{9/2,7/2}$, ..., because they have similar radial wave functions. As it is clear from Eq. (2), a monopole (interaction) matrix element of large magnitude means a larger change of effective SPE. Those changes can give strong impacts on the shell structure throughout the nuclear chart, and such changes of the shell structure are referred to as "shell evolution" [6, 1].

Figure 3 shows typical features of the shell evolution. The single-particle level scheme of Ni isotopes is like the one given by Mayer and Jensen. The strong attraction due to eight protons

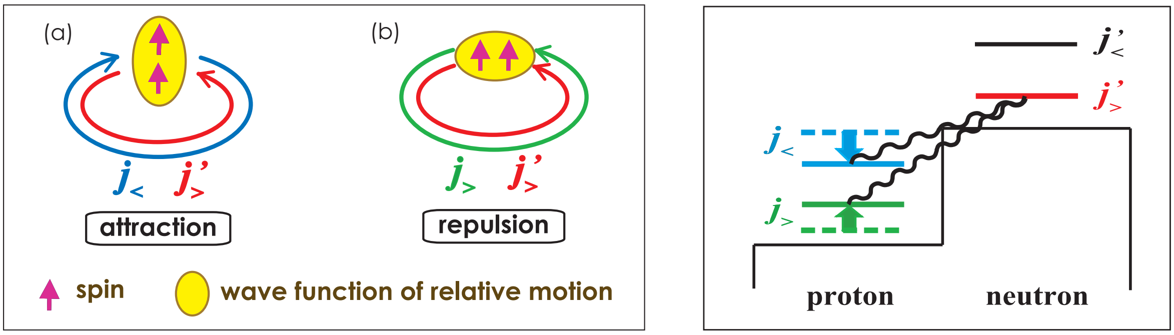

Figure 2. Schematic illustration of the monopole interaction of the tensor force. (Left panel) Attractive and repulsive monopole effects of tensor force. (Right panel) Change of the spin-orbit splitting due to the tensor force and the occupations of the orbit j'. Taken from [6].

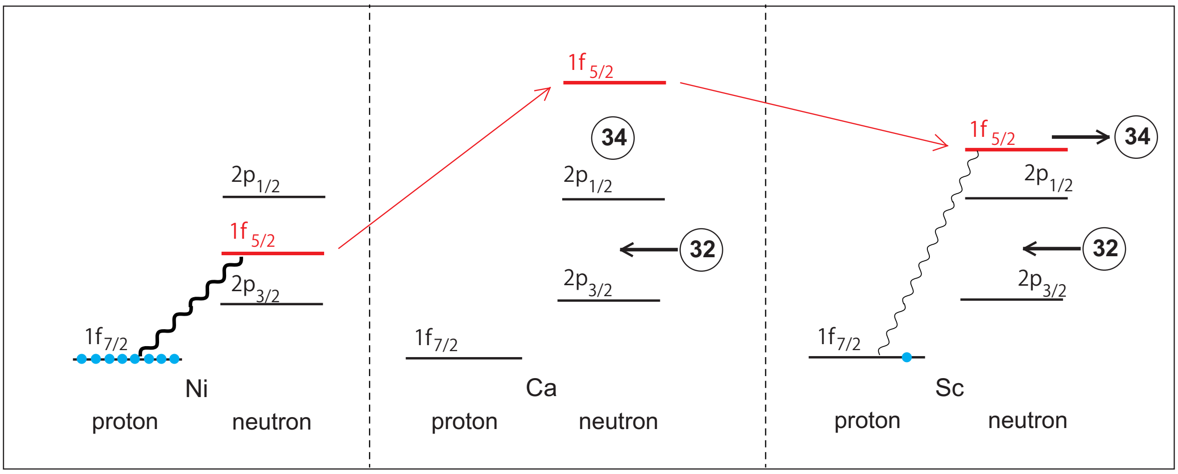

Figure 3. Underlying structure of the single-particle levels of (Left) Ni (Z=28), (Middle) Ca (Z=20) and (Right) Sc (Z=21) nuclei. Level energies are schematic. Wavy lines indicate the interaction between proton in $f_{7/2}$ and neutron in $f_{5/2}$. Thick (thin) wavy line represents stronger (weaker) attraction due to proton(s) in $f_{7/2}$. Numbers in circles are magic numbers. The N=34 magic gap is reduced in Sc isotopes.

keeps the neutron $f_{5/2}$ orbit down between $p_{3/2}$ and $p_{1/2}$ (see Figure 3 (left)). The proton $f_{7/2}$ orbit is vacant in Ca isotopes, and the neutron $f_{5/2}$ orbit loses this attraction, lying high. As it moves above $p_{1/2}$, the N=32 magic gap appears. If the $f_{5/2}$ orbit is high enough, the N=34 magic gap arises.

The N=32 and 34 magic gaps thus emerge. Although the N=32 magic gap was experimentally seen earlier [7], the N=34 magic number followed a different story. It was predicted in 2001 based on a general argument of the spin-isospin interaction [8], but the experiment was so difficult that the 2^+ energy was measured by the rare-isotope beam of the RIBF[9] 12 years later, contrary to the argument in [10].

The above-mentioned mechanism for the N=32 and 34 magic numbers is clearly absent in the "shell model" of Mayer and Jensen, thus leading to new magic numbers. Although the magic gap is not as large as 4 MeV, the closed shell structure has been experimentally confirmed by direct reaction experiments[11].

The mass measurement is another way to confirm the new magic numbers[12]. Figure 3 (Right) indicates how the new magic gaps change if a proton is added in the $f_{7/2}$ orbit (Sc isotopes). The N=34 magic gap fades away immediately, but the N=32 magic gap persists. Quite recently, the masses of Sc isotopes were measured[13], confirming this feature and the underlying idea.

Further studies are on-going about the N=34 magic numbers. The N=34 gap remains for Z =18 (Ar isotopes), but the N=32 gap becomes weaker [14]. These data are included in Fig. 1. Neutron-rich Ca isotopes with more excess neutrons are of great interest also from the viewpoint of the r process. New data and theoretical calculations are coming up, see the talk by S. D. Chen.

The shell evolution has been seen in other nuclei. For instance, the spin-orbit splitting between the neutron $d_{5/2}$ and $d_{3/2}$ orbits increases from ^{35}S to ^{39}Ca due to the tensor force, as seen in an experiment in iThemba-lab (see the talk by O. Sorlin). Without the tensor force, the trend becomes opposite.

The shell evolution thus emerged as one of the major subjects of the Rare-Isotope physics, as addressed also in plenary talks by T. Glasmacher and H. Sakurai. The shell evolution is a new terminology. If one checks it by Google Scholar, there is no hit with "shell evolution" until the year 2003. The Google Scholar shows one first hit for it in 2004. Now you get about 140 hits per year, including those for type-II shell evolution, for instance[15, 16, 17]. (Please combine with something like "atomic nuclei", to avoid contributions from biology or medicine. They discuss a lot on "evolution" and "shell".) There have been so many papers on the shell evolution particularly experimental ones. A good fraction of them were covered in a recent review article [1], but many papers are emerging one after another as indicated by the number of the hits in Google Scholar mentioned above. This is a good sign of healthy developments of nuclear physics, providing a support for constructing various facilities. It is a pity that John P. Schiffer, who made many contributions to the understanding of single-particle states in exotic nuclei (a most recent paper[18]), passed away in 2022.

It is noted that, prior to the shell evolution, earlier empirical analyses were performed by several groups, for example, [19, 20], under different nomenclatures such as "orbital migration".

The tensor force plays crucial roles in the shell evolution. It is natural to include it in the mean field models, as was done by T. H. R. Skyrme in his very original paper for the "Skyrme model" published in 1958 [21]. This spirit was maintained by D. Vautherin and D. M. Brink[22], but no actual inclusion was done because of complexities. A short-range tensor term was proposed by Fl. Stancu, D. M. Brink and H. Flocard (SBF) in 1977 [23], and its application was reported 30 years later [24] probably by some inspiration from [6]. After 2006, many papers were published taking the SBF formulation (see [1] for a review), while a possible insufficient flexibility of the Skyrme model for including the tensor force was discussed in [25]. David Brink kept his keen interest in the tensor force and its effects, but we are sorry that he passed away in 2021. The Gogny force can be extended with the tensor force[26]. Relativistic approaches are making progress. For example, the exchange term (or Fock term) has been included[27] as one of the essential aspects of the tensor force effects[6]. Thus, the approaches by mean-field models and theories show basic feasibilities and expected successes, but the actual tractable formulations are to come.

3. Nuclear shapes

The lower panel of Fig. 1 exhibits new magic numbers, but there is none beyond ^{78}Ni. This is certainly because a strong deformation characterizes the structure of heavy nuclei except for those close to conventional magic numbers. The tensor force, combined with the central force, played major roles in the shell evolution. Does this combination produce no major effects in heavy deformed nuclei? These forces must be there, in action. I will now discuss this natural question now.

The discussion is focused on the nucleus ^{166}Er, although the subject is general. Aage Bohr delivered his Nobel lecture in 1975 [28], showing the level scheme of ^{166}Er. He convincingly argued that the shape of the ground state is an axially-symmetric prolate ellipsoid, and the 2_2^+ state is a γ vibrational excitation. We performed Monte Carlo Shell Model (MCSM) [29] with a large model space with 28 active protons and 28 active neutrons by using a realistic interaction, on the K [30] and Fugaku [31] supercomputers.

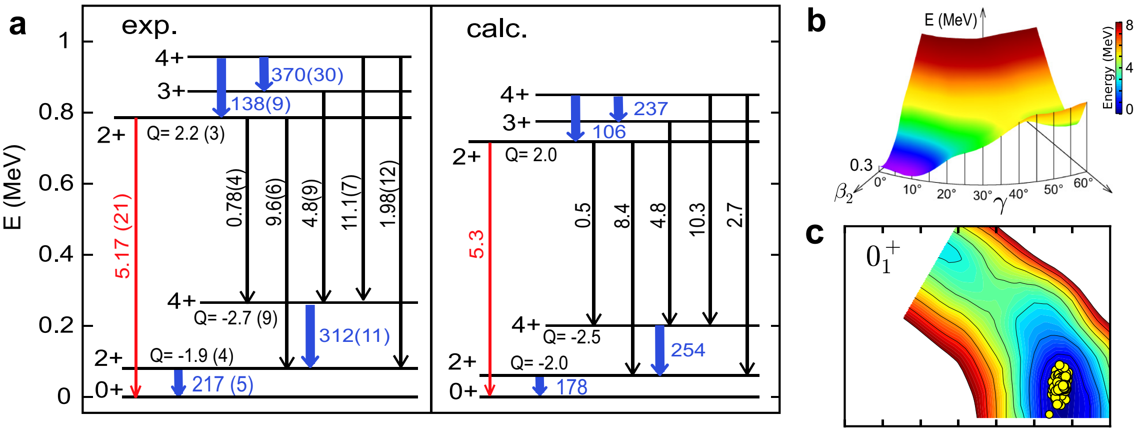

Figure 4. Properties of low-lying states of ^{166}Er. B(E2) values are in W.u. Taken from a part of [29].

Figure 4**a** exhibits the level scheme. The calculation reproduces the ground and so-called γ band rather well in comparison to experiment[32]. Of particular importance is a simultaneous reproduction of the large B(E2)/quadrupole moment values involving the 2_1^+ state, and the smaller $B(E2; 2_2^+ \to 0_1^+)$ value. The latter is about 5 W.u. in both experiment and this theory: this value is larger than simple single-particle estimate, and this observed property is considered to be a signature of the decay of a γ phonon which is collective to a certain extent[28].

The MCSM calculation leads us to a different picture. Figure 4**b** displays the potential energy surface (PES) for the same Hamiltonian. The minimum is not at γ=0, but around γ=10°, which contradicts the idea of the axially-symmetric prolate shape (γ=0) by Aage Bohr [28, 33]. The deviation from the axially symmetry is called triaxiality in general. The triaxiality in ^{166}Er is definitely beyond small fluctuations from γ=0, as it is built on a real minimum. This feature is further examined by the T-plot, which shows individual basis vectors of a given eigen wavefunction. Figure 4**c** depicts the T-plot of the ground state of ^{166}Er, which clearly indicates that the wave function is a superposition of basis vectors around γ=10°. The T-plot was obtained for other eigenstates, 2_1^+, 4_1^+, 2_2^+, 3_1^+, 4_2^+, showing similar patterns. Thus, a rather common triaxiality is evidently seen. This picture is similar to the model of Davydov and his collaborators[34, 35]. The Davydov model assumes a rigid triaxiality, and treats rotational motions of such rigid triaxial object quantum mechanically. It predicted relative B(E2) values well, but failed to reproduce excitation energies of, for instance, the 2_2^+ state and the band built on it [36]. The MCSM wave functions of these low-lying states show similar triaxialities as the Davydov model does, but their excitation energies agree with experiment. A precise treatment of effects of nucleon-nucleon interactions probably makes this difference. Nevertheless, many of rare-earth nuclei show the triaxiality, proving that Davydov's idea is not far from the truth.

The rotation of a rigid triaxial object is likely too naïve.

We recently performed the MCSM calculations by a more advanced methodology called Quasiparticle Vacuum Shell Model[37], which can give us more precise results. But it does not change the present picture for ^{166}Er and surrounding nuclei in the nuclear chart. The underlying mechanism for the triaxiality is then of great interest. In short, the monopole interaction of the tensor force lowers particular couplings, such as proton $h_{11/2}$ and neutron $h_{9/2}$, which enhance the triaxiality with favorable occupation numbers of such single-particle orbits. I mentioned, in the beginning of this talk, a question as to what the tensor force does for heavy nuclei in a visible way, instead of the shell evolution. We can see how this question can be answered. We note that earlier works also pointed out possible deviations from the prolate or phonon-vibrational pictures[38, 39].

4. Final note on Davydov

I note finally that the prevailing triaxiality in heavy nuclei was suggested by a Ukrainian physicist, Dr. A. S. Davydov (Crimea 1912 - Kyiv 1993), but this suggestion was not been well appreciated partly due to excitation energies' discrepancies. Since the basic idea of triaxiality is now shown to be relevant and most likely correct, I believe that Dr. A. S. Davydov and his work can be more appreciated.

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