Frontiers and challenges of nuclear shell model

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Abstract. Two recent developments of the nuclear shell model are presented. One is a breakthrough in computational feasibility owing to the Monte Carlo Shell Model (MCSM). By the MCSM, the structure of low-lying states can be studied with realistic interactions for a wide, nearly unlimited basically, variety of nuclei. The magic numbers are the key concept of the shell model, and are shown to be different in exotic nuclei from those of stable nuclei. Its novel origin and robustness will be discussed.

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1 Introduction

We present two recent developments in the nuclear shell model. One is a drastic change of the feasibility of the shell model calculations due to the Monte Carlo Shell Model. We will discuss this point first by showing several examples. The other is more fundamental: new magic numbers in exotic nuclei. In exotic nuclei far from the β -stability line, some usual magic numbers disappear while new ones arise. This is a very intriguing problem, and its mechanism is related to basic properties of nucleon-nucleon interaction in a very robust way. The second part of this report is on this very exciting and newest development.

2 Monte Carlo Shell Model

2.1 Outlook

The nuclear shell model has been started by Mayer and Jensen in 1949 [1] as a single-particle model. Afterwards, many valence particles are treated in the shell model, which then became a many-body theory or calculational method. A good example can be found in the *sd*-shell [2]. The nuclear shell model has been successful in the description of various aspects of nuclear structure, partly because it is based upon a minimum number of natural assumptions, and partly because all dynamical correlations in the model space, beyond the mean-field calculations, can be incorporated appropriately. Although the direct diagonalization of the Hamiltonian matrix in the full valence-nucleon Hilbert space is desired, the dimension of such a space is too large in many cases, preventing us from performing the full calculations. Indeed, the shell model dimension is large, and the actual calculation becomes very difficult. By recent (conventional) shell model codes like ANTOINE by Caurier [3], VECSSE by Sebe [4] or MSHELL by Mizusaki [5], one can handle up to shell model dimension ~ 100 million at technical edge, while practical calculations up to a few tens million dimension can be done.

Although the conventional shell model calculation has thus been developed significantly, the dimension can be much larger in many real nuclei and is indeed much beyond the reach of future development. For instance, certain unstable nuclei being studied require calculations with more than 1 billion dimension. This is already very far beyond the limit of the existing conventional shell model codes.

In order to overcome those difficulties, one has to introduce an alternative approach. That is, stochastic methods to many-body problems. We now turn to this subject.

The Shell Model Monte Carlo (SMMC) method has been proposed first [6], but it turned out that the SMMC

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is not very suitable for investigating level structure or transitions between eigenstates, partly due to the so-called minus-sign problem.

The Quantum Monte Carlo Diagonalization (QMCD) method has been proposed several years later by Honma, Mizusaki and myself [7]. In the QMCD method, we select only basis states important to the eigenstate to be obtained. We then diagonalize the Hamiltonian matrix in a good approximation with those important bases [8–11]. The application of the QMCD method to the nuclear shell model is called the *Monte Carlo Shell Model (MCSM)*. There have been several publications already on such applications [12–17].

2.2 Features of MCSM

There are two major advantages in the MCSM calculations. The first one is the feasibility of including many single-particle states. Because of this, one can describe drastic excitations within a nucleus. For instance, one can describe spherical yrast states, deformed rotational band and nearly superdeformed band at the same time with the same Hamiltonian in the same model space. This example is shown in refs. [10,12,17], where those three kinds of states are nicely presented by MCSM calculations with the full pf-shell and the $g_{9/2}$ orbit. One finds quite good agreement with experiment [18]. This kind of description over a wide variety of states may be characterized as the feasibility along the energy axis.

The second major advantage of the MCSM calculation is the feasibility of handling many valence particles. The maximum number of valence particles is rather limited in the conventional calculations. However, if one wants to describe a long chain of isotopes entering the region of exotic nuclei far from the β -stability line, the number of particles should change significantly. So, this capability plays an indispensable role in studying the structure of such exotic nuclei. This feature can be characterized as the feasibility along the isospin axis.

The second advantage is essential also in a recent work for describing the spherical-deformed phase transition in heavy nuclei, because the phase transition occurs as a function of the valence nucleons [14].

In exotic nuclei, two major shells are mixed rather often, and states of various characters arise at low energy. Even the ground state can be of quite exotic nature. In this situation, the above two feasibilities combined together play really crucial roles in clarifying the structure of exotic nuclei far from the β -stability line. As an example, we shall discuss the structure of nuclei in the vicinity of ³²Mg in the next section.

3 Magic numbers of exotic nuclei

3.1 Motivation

The magic number is the most fundamental quantity governing the nuclear structure. The nuclear shell model has



Fig. 1. Effective single-particle energies of neutrons of (a) O isotopes for N = 8 to 20 and (b) N = 20 isotones for Z = 8 to 20.

been started by Mayer and Jensen by identifying the magic numbers and their origin [1]. The study of nuclear structure has been advanced on the basis of the shell structure associated with the magic numbers. This study, on the other hand, has been made predominantly for stable nuclei, which are on or near the β -stability line in the nuclear chart. This is basically because only those nuclei have been accessible experimentally. In such stable nuclei, the magic numbers suggested by Mayer and Jensen remain valid, and the shell structure can be understood well in terms of the harmonic-oscillator potential with a spin-orbit splitting.

Recently, studies on exotic nuclei far from the β stability line have started owing to the development of radioactive nuclear beams. The magic numbers in such exotic nuclei can be a quite intriguing issue. We shall show that new magic numbers appear and some others disappear in moving from stable to exotic nuclei in a rather novel manner due to a particular part of the nucleonnucleon interaction.

3.2 Effective single-particle energies

In order to understand underlying single-particle properties of a nucleus, we can make use of *effective (spherical)* single-particle energies (ESPEs), which represent mean effects from the other nucleons on a nucleon in a specified single-particle orbit. The two-body matrix element of the interaction depends on the angular momentum J, coupled by two interacting nucleons in orbits j_1 and j_2 . Since we are investigating a mean effect, this J-dependence is averaged out with a weight factor (2J + 1), and only diagonal matrix elements are taken. Keeping the isospin dependence, T = 0 or 1, the so-called monopole Hamiltonian



Fig. 2. Effective $1s_{1/2}$ - $0d_{3/2}$ gap in N = 16 isotones as a function of Z. Shell model Hamiltonians, SDPF, USD and "Kuo" are used. See the text.

is thus obtained with a matrix element [19, 13]:

$$V_{j_1j_2}^T = \frac{\sum_J (2J+1)\langle j_1 j_2 | V | j_1 j_2 \rangle_{JT}}{\sum_J (2J+1)}, \quad \text{for } T = 0, 1, (1)$$

where $\langle j_1 j_2 | V | j'_1 j'_2 \rangle_{JT}$ stands for the matrix element of a two-body interaction, V.

The ESPE is evaluated from this monopole Hamiltonian as a measure of mean effects from the other nucleons. The normal filling configuration is used. Note that, because the J-dependence is taken away, only the number of nucleons in each orbit matters. As a natural assumption, the possible lowest isospin coupling is assumed for protons and neutrons in the same orbit. The ESPE of an *occupied* orbit is defined to be the separation energy of this orbit with the opposite sign. Note that the separation energy implies the minimum energy needed to take a nucleon out of this orbit. The ESPE of an *unoccupied* orbit is defined to be the binding energy gain by putting a proton or neutron into this orbit with the opposite sign.

3.3 Varying shell gaps

In fig. 1(a), ESPEs are shown for O isotopes. The Hamiltonian and the single-particle model space are the same as those used in Utsuno *et al.* [13], where the structure of exotic nuclei with $N \sim 20$ has been successfully described within a single framework.

A significant gap is found at N = 16 with the energy gap between the $0d_{3/2}$ and $1s_{1/2}$ orbits equal to about 6 MeV. This is a quite large gap comparable to the gap between the *sd*- and *pf*-shells in ⁴⁰Ca. The neutron number N = 16 should show features characteristic of magic numbers as pointed out by Ozawa *et al.* [20] for observed binding energy systematics. A figure similar to fig. 1(a) was shown by Brown [21] for the USD interaction [2],



Fig. 3. ESPEs for (a) ³⁰Si and (b) ²⁴O, relative to $0d_{5/2}$. (c) The major interaction producing the basic change between (a) and (b). (d) The process relevant to the interaction in (c).

while only nuclei with subshell closures were taken. Basically because the $0d_{3/2}$ orbit has positive energy as seen in fig. 1(a), O isotopes heavier than ²⁴O are unbound for the present Hamiltonian in agreement with experiments [22, 23], whereas the $0d_{3/2}$ orbit has negative energy for the USD interaction [2,21].

One finds that the gap between the $0d_{3/2}$ and $1s_{1/2}$ orbits is basically constant within a variation of $\sim \pm 1$ MeV. In lighter O isotopes, valence neutrons occupy predominantly $0d_{5/2}$ and this gap does not make much sense to the ground or low-lying states. The gap becomes relevant to those states only for N > 14. Thus, the large $0d_{3/2}$ - $1s_{1/2}$ gap exists for O isotopes in general, while it can have major effects on the ground state for heavy O isotopes, providing us with a magic nucleus ²⁴O at N = 16.

Figure 2 shows the effective $0d_{3/2}$ - $1s_{1/2}$ gap, *i.e.*, the difference between ESPEs of these orbits, in N = 16 isotones with Z = 8-20 for three interactions: "Kuo" means a *G*-matrix interaction for the *sd*-shell calculated by Kuo [24], and USD was obtained by adding empirical modifications to "Kuo" [2]. The present shell model interaction is denoted SDPF hereafter, and its *sd*-shell part is nothing but USD with small changes [13]. Steep decrease of this gap is found in all cases, as *Z* departs from 8 to 14. In other words, a magic structure can be formed around Z = 8, but it should disappear quickly as *Z* deviates from 8 because the gap decreases very fast. The slope of this

sharp drop is determined by $V_{0d_{5/2}0d_{3/2}}^{T=0,1}$ in eq. (1), where the dominant contribution is from T=0.

The gap can be calculated from the Woods-Saxon potential. The resultant gap is rather flat, and is about half of the SDPF value for Z = 8.

3.4 Shell structures of ³⁰Si and ²⁴O

We now discuss, in more detail, the sharp drop of the gap indicated in fig. 2 for Z moving away from 8. This drop is primarily due to the rapid decrease of the $0d_{3/2}$ ESPE for neutrons. Figure 3 shows ESPEs for ³⁰Si and ²⁴O, both of which have N = 16. Note that ³⁰Si has six valence protons in the *sd* shell on top of the Z = 8 core and is indeed a stable nucleus, while ²⁴O has no valence proton in the usual shell model. In fig. 3, the neutron $0d_{3/2}$ and $1s_{1/2}$ are rather close to each other, while keeping certain gaps from the other orbits. Thus, the $0d_{3/2}$ - $1s_{1/2}$ gap becomes smaller as seen in fig. 3(a).

In fig. 3(b), ESPEs for an exotic nucleus, ²⁴O are shown. The $0d_{3/2}$ is lying much higher, very close to the pf-shell. A considerable gap (~ 4 MeV) is between the $0d_{3/2}$ and the pf-shell for the stable nucleus ³⁰Si, whereas an even larger gap (~ 6 MeV) is found between $0d_{3/2}$ and $1s_{1/2}$ for ²⁴O. The basic mechanism of this dramatic change is the strongly attractive interaction shown schematically in fig. 3(c), where $j_{>} = l + 1/2$ and $j_{<} = l - 1/2$, with l being the orbital angular momentum. In the present case, l = 2. One now should remember that valence protons are added into the $0d_{5/2}$ orbit as Z increases from 8 to 14. Due to a strong attraction between a proton in $0d_{5/2}$, a neutron in $0d_{3/2}$, as more protons are put into $0d_{5/2}$, a neutron in $0d_{3/2}$ is more strongly bound. Thus, the $0d_{3/2}$ ESPE for neutrons is so low in ³⁰Si as compared to that in ²⁴O.

3.5 Spin-isospin dependence in NN interaction

The process illustrated in fig. 3(d) produces the attractive interaction in fig. 3(c). The NN interaction in this process is written as

$$V_{\tau\sigma} = \tau \cdot \tau \ \sigma \cdot \sigma \ f_{\tau\sigma}(r). \tag{2}$$

Here, the symbol "." denotes a scalar product, τ and σ stand for isospin and spin operators, respectively, r implies the distance between two interacting nucleons, and $f_{\tau\sigma}$ is a function of r. In the long-range (or no r-dependence) limit of $f_{\tau\sigma}(r)$, the interaction in eq. (2) can couple only a pair of orbits with the same orbital angular momentum l, which are nothing but $j_>$ and $j_<$.

The σ operator couples $j_>$ to $j_<$ (and vice versa) much more strongly than $j_>$ to $j_>$ or $j_<$ to $j_<$. Therefore, the spin-flip process is more favored in the vertices in fig. 3(d). The same mathematical mechanism works for isospin: the τ operator favors charge exchange processes. Combining these two properties, $V_{\tau\sigma}$ produces large matrix elements for the spin-flip isospin-flip processes: proton in $j_> \rightarrow$ neutron in $j_<$ and vice versa. This gives rise to the interaction in fig. 3(c). This feature is a general one and is maintained with $f_{\tau\sigma}(r)$ in eq. (2) with reasonable *r*-dependences.

Although $V_{\tau\sigma}$ yields sizable attraction between a proton in $j_{>}$ and a neutron also in $j_{>}$, the effect is weaker than in the case of fig. 3(c).

In stable nuclei with $N \sim Z$ with ample occupancy of the $j_{>}$ orbit in the valence shell, the proton (neutron) $j_{<}$ orbit is lowered by neutrons (protons) in the $j_{>}$ orbit. In exotic nuclei, this lowering can be absent, and then the $j_{<}$ orbit is located rather high, not far from the upper shell. In this sense, the proton-neutron $j_{>}-j_{<}$ interaction enlarges a gap between major shells for stable nuclei with proper occupancy of relevant orbits.

The origin of the strongly attractive $V_{\tau\sigma}$ is quite clear. The One-Boson-Exchange-Potentials (OBEP) for π and ρ mesons have this type of terms as major contributions. While the OBEP is one of major parts of the effective NN interaction, the effective NN interaction in nuclei can be provided by the *G*-matrix calculation with core polarization corrections. Such effective NN interaction will be called simply *G*-matrix interaction for brevity. The *G*matrix interaction should maintain the basic features of meson exchange processes, and, in fact, existing *G*-matrix interactions for the cases shown in fig. 3(c) [25].

We would like to point out that the $1/N_c$ expansion of QCD by Kaplan and Manohar indicates that $V_{\tau\sigma}$ is one of three leading terms of the NN interaction [26]. Since the next order of this expansion is smaller by a factor $(1/N_c)^2$, the leading terms should have rather distinct significance.

3.6 Disappearance of $\mathsf{N}=20$ magic structure: same origin

We now turn to exotic nuclei with $N \sim 20$. The ESPE has been evaluated for them in [13]. Narrow effective gap for neutrons between $0d_{3/2}$ and the pf-shell is obtained for exotic neutron-rich nuclei with $N \sim 20$ as can be seen in fig. 1(b). Such a small gap is found to play an essential role for various anomalous features. This small gap is nothing but what we have seen for ²⁴O in fig. 3(b). Thus, the disappearance of N = 20 magic structure in Z = 9-14 exotic nuclei and the appearance of the new magic structure in ²⁴O have the same origin.

The Monte Carlo Shell Model has been applied to the structure study of extremely neutron-rich unstable nuclei around ³²Mg [13]. Since the major issue is the breaking of the N = 20 closed shell, one has to include both the *sd*-shell and the *pf*-shell. In fact, because of narrower effective shell gap near Z = 10 as discussed above, intruder configurations come down and are mixed with normal configurations. The intruder configurations come down also because they are more deformed and can gain more T = 0 correlation energies the large part of which is quadrupole deformation energy. A large deformation can be expected for Mg and Ne isotopes. These two mechanisms, narrower gap and stronger deformation, are combined and produce intriguing properties [13,27–29,3,30–33].

3.7 Magic numbers in the p-shell: N = 6 vs. N = 8

A very similar mechanism works for *p*-shell nuclei. The neutron $0p_{1/2}$ orbit becomes higher as the nucleus loses protons in its spin-flip partner $0p_{3/2}$. The N = 8 magic structure then disappears, and N = 6 becomes magic, similarly to N = 16 magic number in the *sd*-shell. As a consequence, ⁸He is well bound, whereas ⁹He is not bound. This is analogous to the situation that ²⁴O is well bound, but ²⁵O is unbound.

3.8 Heavier nuclei: N = 34, etc.

Moving back to heavier nuclei, from the strong interaction in fig. 3(c), we can predict other magic numbers, for instance, N = 34 associated with the $0f_{7/2}$ - $0f_{5/2}$ interaction. In heavier nuclei, $0g_{7/2}$, $0h_{9/2}$, etc. are shifted upward in neutron-rich exotic nuclei, disturbing the magic numbers N = 82, 126, etc. It is of interest how the r-process of nucleosynthesis is affected by it.

3.9 Summary of the section

In summarizing this section, we showed how magic numbers are changed in nuclei far from the β -stability line: N = 6, 16, 34, etc. can become magic numbers in neutronrich exotic nuclei, while usual magic numbers, N = 8, 20,40, etc., may disappear. Since such changes occur as results of the nuclear force, there is isospin symmetry that similar changes occur for the same Z values in mirror nuclei. The mechanism of this change can be explained by the strong attractive $V_{\tau\sigma}$ interaction which has robust origins in OBEP, G-matrix and QCD. In fact, a simple structure such as magic numbers should have a simple and sound basis. Since it is unlikely that a mean central potential can simulate most effects of $V_{\tau\sigma}$, we should treat $V_{\tau\sigma}$ rather explicitly. It is nice to build a bridge between the very basic feature of exotic nuclei and the basic theory of hadrons, QCD. In existing Skyrme HF calculations, except for those with Gogny force, effects of $V_{\tau\sigma}$ may not be well enough included, because the interaction is truncated to be of δ function type. The Relativistic Mean Field calculations must include pion degrees of freedom to be consistent with $V_{\tau\sigma}$. Thus, the importance of $V_{\tau\sigma}$ opens new directions for mean-field theories of nuclei. Loose-binding or continuum effects are important in some exotic nuclei. By combining such effects with those discussed in this talk, one may draw a more complete picture for the structure of exotic nuclei. Finally, we would like to mention once more that the $V_{\tau\sigma}$ interaction should produce large, simple and robust effects on various properties, and may change the landscape of nuclei far from the β -stability line in the nuclear chart.

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