Notes

Approaching a mystery of doubly closed shell in nuclei

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- We have studied the nuclear structure around a doubly closed-shell nucleus ^{16}O with large-scale shell-model calculations, aiming at clarifying the mechanism of the appearance of excited states in the low excitation energy region.
- We have found that the excited states are lowered by the significant reduction of the shell gap from the so-believed "experimental gap," on the assumption of the independent-particle model in fact, due to the correlation energy.
- This result leads to a renewed understanding of the closed-shell structure, and indicates that the excited states of closed-shell nuclei can be described with an extended independent-particle picture.

Abstract

It has been widely accepted that the excited states of doubly-closed shell nuclei, which has a closed-shell configuration for both protons and neutrons, are located high because of the stability of the closed-shell structure. In a doubly-closed nucleus ^{16}O, however, there exists an excited state having much lower excitation energy than a simple estimate from the closed-shell structure. While the state is regarded as the one dominated by four-particle four-hole excitation from the closed-shell configuration, the mechanism of the lowering has not been clear from the viewpoint of microscopic theories, most of which give the excitation energy more than twice as high as the experimental value. In the present study, we have found that the shell gap for ^{16}O is much reduced from the value deduced straightforwardly from experiment with the independent-particle picture, which leads to a successful description of the location of the excited state within the framework of large-scale shell-model calculations. This result gives a renewed picture about the shell structure, one of the most basic properties in nuclei. The present work has been published in Physical Review C [1].

1. Background of the study

It is a well-known fact that diversity and periodicity of atomic properties are dominated by electrons each of which occupies an independent quantized orbit. In a similar way, the independent-particle picture is

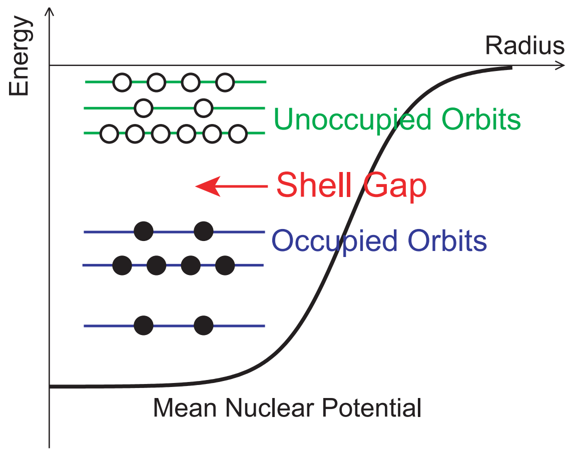

Fig.1. Schematic illustration of the closed-shell structure. If large energy difference (called the shell gap) exists between unoccupied orbits and occupied orbits made by a mean nuclear potential, the nucleus is especially stable because large energy is needed to excite a particle in the occupied orbit (filled circle) into the unoccupied orbit (open circle).

believed to work quite well in nuclei: nucleons, i.e., protons and neutrons that constitute a nucleus, are dominated by a mean potential which is created by the nucleus itself. This picture leads to various basic properties of nuclei. For instance, nuclei with the so-called magic number need more energy to excite than surrounding nuclei because they have closed-shell configurations as illustrated in Fig. 1. This situation exactly corresponds to rare-gas elements, which are chemically quite inactive, in atoms. It is due to the closed-shell structure formed at proton number

(Z) 82 that all nuclei having more protons than lead (Z=82), such as polonium (Z=84) and radium (Z=88) discovered by Pierre and Marie Curie, are unstable against the emission of an α particle. In addition, the smallest magic number two accounts for the reason why those nuclei emit nothing but the α particle, the ^{4}He nucleus comprising two protons and two neutrons.

Although especially stable are the nuclei whose protons and neutrons form the closed shell, referred to as the doubly-closed shell nuclei or doubly-magic nuclei, some of their excited states are not described by the simple independent-particle picture. For instance, this picture hardly accounts for the spin-parity quantum number of the first excited state of a doubly-magic nucleus ^{16}O (eight protons and eight neutrons) located at 6.05 MeV, 0^{+}, because it cannot be realized by a one-particle one-hole excitation from the closed-shell configuration. While this state is considered to be dominated by a four-particle (α particle) excitation across the shell gap, it has not been still quantitatively clarified what pulls down the state as low as ~6 MeV overwhelming the shell gap of ~10 MeV. The present study is thus aimed at giving its solution.

Since, as seen above, the nuclear structure shows various aspects which are based on but sometimes deviate from the independent particle picture, current nuclear theory is progressing to understand the diversity in the wide-spreading nuclear chart including neutron-rich nuclei and hypernulei from a microscopic point of view. For this purpose, one has to revisit the basis and validity of assumptions adopted before.

2. Circumstances of the study

The key of the present study is the shell structure. Following my belief that those who govern the shell structure govern the nuclear structure, I have been studying the mechanism of the appearance of exotic shell structure seen in neutron-rich nuclei and its impact on the many-body problem in nuclei. The present research started when the following presumption of the shell structure was taken into consideration.

It is widely accepted that the single-particle energies of the occupied and unoccupied orbits in ^{16}O are determined from experiment. Namely, as displayed in Fig. 1, the binding energy of the highest occupied orbit is identical with the one-neutron separation energy of ^{16}O, $Sn(^{16}\mathrm{O})$, and that of the lowest unoccupied orbit is $Sn(^{17}\mathrm{O})$. Corresponding to the Koopmans' theorem in the atomic physics [2], this holds exactly in the context of the simplest independent-particle model based on the independent-particle picture. The shell gap is thus derived from $Sn(^{17}\mathrm{O})-Sn(^{16}\mathrm{O})$, which amounts to 11.5 MeV. The single-particle energies of doubly-magic nuclei carry much information about determining parameters of phenomenological mean-field models.

While the independent-particle picture is a fairly good approximation in nuclei, one should not neglect the effect of the two-body force that is not incorporated in the mean potential and is thus called the residual interaction. In the ^{16}O case, the total many-body system is more stabilized, or equivalently, its energy is lowered by scattering part of nucleons in occupied orbits into unoccupied orbits by means of the two-body force. It is hardly accepted in the classical mechanics but is realized in the quantum mechanics as a result of the superposition principle that the total energy is lowered by exciting particles into higher orbits. The energy gained by breaking the closed shell is referred to as the correlation energy in contrast to the independent or "uncorrelated" particle. As shown in the next section in detail, the new finding of the present study is that the correlation energy plays an essential role both in the closed-shell formation in ^{16}O and in its excitation.

Although the importance of the correlation energy is recognized for open-shell nuclei (i.e. non-closed-shell nuclei), its influence on closed-shell nuclei has not been taken seriously due to the success of the independent-particle picture. By remembering that the one-neutron separation energy is identified with the single-particle energy in the independent-particle model, if the correlation energy exists but it is common over an isotope chain, the contribution of the correlation energy to the separation energy is cancelled and the Koopmans' theorem still holds. I suppose that those facts constitute the reason for the ignorance of the correlation energy in previous studies.

3. Contents of the study

Firstly, we evaluate the correlation energy using large-scale shell-model calculations. The shell model including configuration mixing is characterized as a model which is most faithful to the quantum mechanics for a quantum many-body problem having a given set of single-particle orbits, and is equivalent to the configuration interaction (CI) method in the quantum chemistry. Since this is an approach exactly

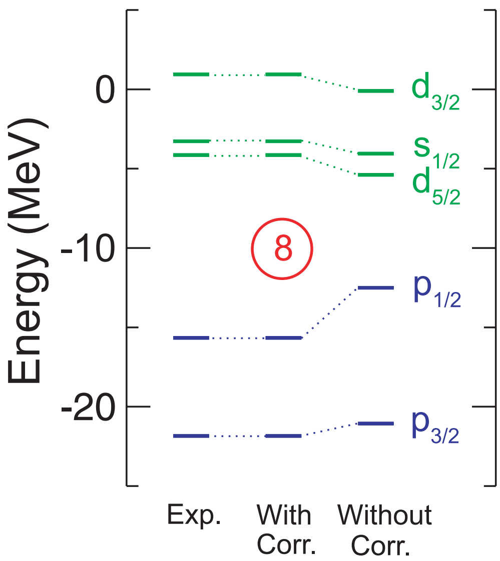

Fig.2. Single-particle-like spectra around ^{16}O compared between experiment and theory. The experimental levels (left) are taken from those of ^{15}O and ^{17}O. So as to reproduce them including correlation energy (center), the single-particle (uncorrelated) energies shown in the rightmost column should be taken.

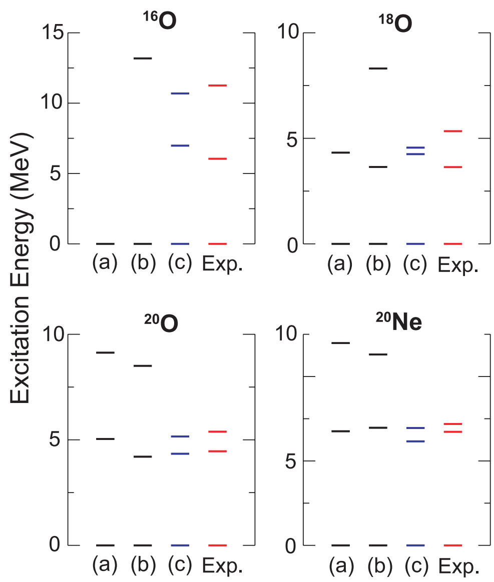

Fig.3. The lowest three 0$^+$ energy levels in ^{16,18,20}O and ^{20}Ne compared between experiment (Exp.) and theory. (a) Calculation without excitation from the *p* shell to the *sd* shell. (b) Calculation with the excitation using the single-particle energies of the independent-particle model. (c) Calculation with the excitation using the corrected single-particle energies by taking into account the correlation energy.

treating many-body effects, the correlation energy can be obtained once a reasonable set of occupied and unoccupied orbits is taken as the model space and an appropriate Hamiltonian (i.e., an energy operator to obtain many-body states) is provided. Here, we adopt the model space that fully allows the excitation of nucleons in the occupied orbits between magic numbers 2 and 8 (called the *p* shell) into the unoccupied orbits between magic numbers 8 and 20 (called the *sd* shell). The Hamiltonian adopted in this study is a phenomenological one often used in this mass region [3], and its single-particle energy is determined so as to fit the experimental “single-particle spectra” around ^{16}O such as low-lying states of ^{15,17}O within the independent-particle approximation.

When correlation energies are calculated with the above setting, the ground state of ^{16}O reaches 9.4 MeV, which is larger than the values of the ground states of ^{15}O and ^{17}O amounting to 7.2 MeV and 8.4 MeV, respectively. Note that the correlation energy is here defined by additional energy gain having a positive sign. Since the one-neutron separation energy is defined by the difference in energy between neighboring nuclei, $Sn(^{16}\mathrm{O})$ increases by $9.4-7.2=2.2$ MeV and $Sn(^{17}\mathrm{O})$ decreases by $9.4-8.4=1.0$ MeV. In total, $Sn(^{16}\mathrm{O})-Sn(^{17}\mathrm{O})$ increases by 3.2 MeV. This indicates that the correlation energy accounts for about 3 MeV of $Sn(^{16}\mathrm{O})-Sn(^{17}\mathrm{O})$, total of which is due to the shell-gap energy in the independent-particle model. Hence, it is most likely that the shell gap must be reduced by this amount to reproduce the observed energies.

This reduction of the shell gap is estimated more quantitatively. The single-particle energy of the original Hamiltonian [3] is identified with the separation energy on the basis of the independent-particle approximation, replaced by its experimental value. Since the correlation energy brings about deviation in separation energy, the single-particle energies, which are not observables, must be refitted in order to reproduce the separation energies within the framework incorporating the correlation energy. The single-particle energies, i.e., the energies of uncorrelated approximation, are thus corrected as shown in the rightmost column of Fig. 2. As expected already, the correct shell gap is significantly reduced from the so-called experimental value that is straightforwardly deduced from experimental one-neutron separation energies with the independent-particle model.

When the shell gap is reduced, excitation across the gap is more favored in energy, or equivalently, its excitation energy is lowered as expected. Figure 3 compares the 0$^+$ energy levels for nuclei around ^{16}O between experiment and theory. Since Fig. 3 (a) shows the energy levels without excitation across the shell gap, missing states in Fig. 3 (a) corresponds to the state involving such excitation. In the case of ^{16}O, only the ground state appears. When the excitation across the shell gap is allowed with the original Hamiltonian [3], excited states emerge but their excitation energies are much higher than experimental value 6.05 MeV as shown in Fig. 3 (b). On the other hand, experimental energy levels are satisfactorily reproduced with the single-particle energies shown in the rightmost column of Fig. 2, which are determined to fit experimental separation energies including correlation energy. Similarly, the reduced shell gap successfully reproduces the excitation energies of the other nuclei that have sharply deviated in previous calculations.

The above-mentioned narrowed shell gap is caused essentially by the correlation energy peaked at the doubly-magic nucleus ^{16}O. Since there is no space left to discuss its origin, those who are interested in it are referred to [1]. This paper also points out that the correlation energy behaves in a different way depending on the origin of closed-shell formation: whereas it is maximized in the *L-S* closure such as ^{16}O, it is minimized in the *j-j* closure such as ^{56}Ni.

4. Importance of the result and its impact

It was speculated that the first excited state of ^{16}O was dominated by the excitation of a cluster of four nucleons called the α cluster and was difficult to describe with models starting from the mean potential. This study demonstrates that this state can be well described within the single-particle space of satisfactory number of orbits. This leads to the possibility of a unified description of various nuclear structures with the configuration-mixing shell model, which is a natural extension of the independent particle model.

I consider that the narrowed shell gap due to correlation energy will have a great impact on the mean-field model (or the energy density functional method), which is currently a popular model in the nuclear structure study. The parameters taken in the mean-field model are determined so as to fit several observables, one of which is the single-particle energy in the doubly-closed shell nuclei. A previous study suggested [4] that it was difficult to fit the experimental single-particle energies of the *L-S* closed shell nuclei ^{16}O and ^{40}Ca within reasonable parameter sets. Since the present study have indicated that correct theoretical single-particle energies are sharply shifted from the experimental single-particle-like spectra, this problem has been resolved.

5. Perspectives

Towards a unified microscopic description of the nuclear structure, I will develop methodology for describing the structure of heavier nuclei, on the basis of which I will also pursue fundamental principles that govern the many-body properties of nuclei. As for the methodology, a new method called the Monte Carlo shell model [5] will be advanced in order to obtain a precise many-body wave function for a system to which the conventional computing method is not practically applicable. Its progress will enable us to clarify the structure of the next doubly-closed shell nucleus ^{40}Ca in the near future, in particular the coexistence of spherical, deformed and superdeformed states and its relation to the breaking of the closed-shell structure. As for the basic principles, focus will be on exotic properties of nuclei far from stability, which are artificially produced by an accelerator or a reactor, from the viewpoint of the shell structure evolving from stable to unstable nuclei. The present study is a milestone in both directions.

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