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Preliminary Study on Uncertainty of Central Force and Effect of Cross-Shell Excitation in Shell Model

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Abstract: The uncertainty of the nuclear shell model is important but rarely investigated. The present work provides preliminary investigations on the uncertainty of the nuclear force and the effect model space in shell-model calculations. The most important part of the nuclear force is the central force, which is also considered to include the largest contribution from the renormalization effect. If semi-magic nuclei are considered and only the strength of the central force varies, C10 (T,S=1,0) and C11 (T,S=1,1) channels of the central force contribute to the theoretical variances of the description of the levels, while the spin-orbit force and the tensor force are kept unchanged as the bare ones. One set of the strengths of a simple nuclear force gives an 0.2 MeV root mean square (RMS) between observed and theoretical levels from 188 states in Pb and Sn isotopes and N=82 and 126 isotones. However, if levels in these isotopes and isotones are separately considered, RMS are further reduced and found to have two minimums with 15% stronger *pp* interaction than *nn* interaction, which indicates a "mirror difference" in medium and heavy nuclei. The enlarge of the model space are of great significance for the description of certain nuclei, such as the inclusion of cross-shell excitations for the nuclei with magic neutron and/or proton numbers. The neutron-rich F isotopes are investigated through three Hamiltonians. Despite the different results among Hamiltonians, the two neutron separation energies and levels are sensitive to and similarly contributed by the cross-shell excitations.

Key words: shell model; uncertainty; central force; cross-shell excitation
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1 Introduction

The estimation of the uncertainty of a theoretical model is critical for the evaluation of the predictive power of the model[1]. Recent years, the uncertainties of many nuclear models are investigated, including macroscopic, microscopic, and macroscopic-microscopic models, such as the liquid drop model[2–3], the energy density functional theory[4], and the Weizsäcker-Skyrme mass model[5]. However, the uncertainty is rarely studied for the nuclear shell model, which is one of the most important nuclear models. Recently, a quantification of shell-model uncertainty is proposed for p shell[6].

In nuclear shell model, the eigenvalues of the binding energies of both the ground and excited states are simultaneously obtained through solving the many-body Schrodinger equation in a specified model space. The chosen of the model space and the construction of the Hamiltonian for the model space are two key points for shell-model investigations[8]. With proper selections of the Hamitonians and model spaces, the nuclear shell model can be used to investigate the nuclear structure properties from stability line to the drip line and from light to heavy nuclei, including binding energies, levels, electromagnetic properties, β decay properties[7–8]. For example, the mass, B(GT) strength, and branching ratio of ^{22}Si are recently observed and well described by the shell-model calculations when the weakly bound effect is included[9]. The shell-model calculation well reproduces the positions of the band heads of a chiral-like pair band and a six-nucleon noncollective oblate isomer in ^{120}I[10]. The spin parity of the ground state of the newly discovered

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nuclide, ^{223}Np, is suggested to be $9/2^-$ through the combination of the observed α decay width and the shell-model results[11].

It is expected that the shell-model predictions, especially with uncertainties, can contribute to the evaluation of nuclear data, which are of key significance for astrophysics and nuclear engineering. But many useful nuclear data can not be measured in the near future, because these data correspond to extreme conditions, such as extremely neutron (proton)-rich nuclei, high excitation energies, short lifetimes, which are beyond the present ability of the facilities. The requirements on the nuclear structure data are similar for astrophysics and nuclear engineering, which are the nuclear masses, the half-lives, the transition rates and branching ratios of β decay, the ratios of β delayed (two) neutron decay, the spectroscopic factors, and the two-nucleon amplitudes. The neutron-rich fission products around A=140 are also on the r-process and important both in astrophysics and nuclear engineering. The levels of ^{140}Te[12] and the Gamow-Teller transitions of ^{140}I[13] are measured recently through EURICA collaboration.

Recently, the new era of multi-messenger observations started after the observation of a binary neutron star merger[14]. The γ-ray burst was observed for the neutron-star merger, which indicated the synthesis of r-process elements[15]. Such observation provides new insights in understanding the long standing problem, the origin of the element beyond iron. Comparing with the huge reactor, universe, many small reactors are running around the world. Many important properties of actinides and fission products are not (well) measured. More accurate predictions on these data are helpful for many investigations on nuclear energy, such as the transmutation of minor actinides[16–17], the radial properties inside a fuel rod[18–19], and the neutronic properties of the accidental tolerant fuel-cladding combination[20]. It should be helpful to understand these phenomena if the nuclear data on N=82 (126) isotones and fission products are evaluated through the shell model.

Although it is impossible to study all nuclei because of the computational limitation, it is worth to perform systematic shell-model investigation and evaluate its uncertainty from stability line to drip line and from light to heavy nuclei. The present work provides some preliminary discussions on the uncertainties of the nuclear force and the effect of the model space. The investigations on the strength of nuclear force and its uncertainty are long standing topics. But it is still difficult to constrain the strengths of certain terms because of the large uncertainties[21]. The present work try to discuss the sensitivity of central force on the levels from the most simple cases, semi-magic nuclei. It is important to increase the model space to include the cross-shell excitations in the calculation of certain nuclei with neutron or proton numbers around classical magic numbers, especially when the corresponding shell gaps are weakened or disappeared. For example, the ground states of nuclei in “island of inversion” are dominated by the cross-shell configurations. The recent measurement on ^{34}Si shown the transition structure across the northern boundary of “island of inversion”[22]. The present works try to show the importance of the cross-shell excitations in the southern part of “island of inversion”, F isotopes.

2 Hamiltonians

A shell-model Hamiltonian needs to be constructed for shell-model calculations after the selection of the model space. The shell-model Hamiltonians can be obtained through the realistic nuclear force and the phenomenological nuclear force. In the latter case, the strengths of the phenomenological nuclear force are normally fixed to the observed levels, while two ways can be chosen, matrix elements fit (such as WBT[23]) and potential fit (such as WBP[23]). It is more convenient to choose potential fit to investigate the uncertainty of the strength of the phenomenological nuclear force because there are huge amount of matrix elements in the model space with many orbits.

The phenomenological nuclear force, monopole based universal interaction, $V_{\rm MU}$[24], is chosen as the phenomenological nuclear force in the present work. Because $V_{\rm MU}$ only includes central and tensor parts, spin-orbit part of M3Y interaction[25] is also included. The validity of $V_{\rm MU}$+LS(M3Y) is examined in many regions, such as *psd* region[26], *sdpf* region[27], ^{132}Sn region[28], and ^{208}Pb region[29]. At present, only semi-magic nuclei are considered to simplify the problem. In such case, only $T=1$ channel of the nuclear force is needed and written as C10+C11+T1+LS1, where C10 and C11 are T,S=1,0 and T,S=1,1 channels of the central force in $V_{\rm MU}$+LS(M3Y), respectively. T1 and LS1 are T=1 channel of tensor force in $V_{\rm MU}$+LS(M3Y) and T=1 spin-orbit force in M3Y, respectively.

Both the cross-shell configurations and the cross-shell interactions are important for the investigations of the nuclear properties related to cross-shell excitations. In the construction of the *psd* region Hamiltonian, YSOX, 0∼3 $\hbar\omega$ cross-shell excitations are considered, while a weaker off-diagonal cross-shell interaction is found to be necessary to reproduce the binding energies of C, N, O isotopes[26]. The recent observations of the cross-shell states with negative parity in ^{17,19}C are better reproduced by YSOX rather than other Hamiltonians[30]. YSOX also gives nice descriptions on the *sd* cross-shell components in the ground and excitation states in ^{12}Be[31–32]. The levels, electromagnetic transitions, and Gamow-Teller transitions of ^{14}C are well reproduced only when the $4\hbar\omega$ excitation and the weaker off-diagonal cross-shell interaction are both considered[33].

Just beyond C, N, and O isotopes, of which the drip line locates at N=16, F isotopes extend much longer to cross N=20 shell gap. The cross-shell excitations are expected to be significant in neutron-rich F isotopes. Some Hamiltonians are constructed for *sdpf* region, such as SDPF-M[34], SDPF-MU[27], and SDPF-USI[35]. It is worth to investigate the cross-shell excitations through the present Hamiltonians and compare the results among them. All shell model calculations are performed through the code KSHELL[36].

3 "Mirror difference" in medium and heavy nuclei

As a simple assumption, all renormalization effect of the bare nuclear force is considered in the central part. That is to say, the spin-orbit and tensor force are kept as the bare nuclear force in the shell-model calculations, which is examined to be validate for the tensor part[24]. In the present work, only the strength of the central force is changed to simplify the problem. The strengths of C10 and C11 various from 90% to 120% of their original values listed in Ref. [24].

The mirror symmetry is generally kept in mirror nuclei, of which the levels are quite similar. The isospin asymmetry term is weak for nuclear force, while the *pp*, *nn*, and *pn* interactions are quite similar to each other. Some large mirror differences are found in *sd* region, which come from the weakly bound effect[39]. In medium and heavy nuclei, there are no mirror nuclei because neutron numbers are more than proton numbers. However, a "Mirror difference" can be defined if the strength of nuclear force is considered. Taking ^{214}Pb and ^{214}Ra as examples, the former has six neutrons outside doubly magic nucleus ^{208}Pb, while the latter has six more protons. Their levels have no mirror symmetry because the neutrons and protons locate in different orbits. But the strengths of the *nn* and *pp* interactions can be deduced from their levels and show the "Mirror difference", which means the differences between the strengths of *nn* and *pp* interactions in one region.

From Fig. 1, it is clearly seen that the original strength of C10 channel of the central force can well reproduce the level of ^{214}Pb. However, an enhancement of the strength of the C10 channel is needed to reproduce the level of ^{214}Ra, which means the deduced strengths of *nn* and *pp* interactions may be different in ^{208}Pb region. During the changing of the strength of C10 channel, the C11 channel is kept the same as Ref. [24]. The C11 channel has almost no impact on the levels of ^{214}Pb and ^{214}Ra, which will be discussed later.

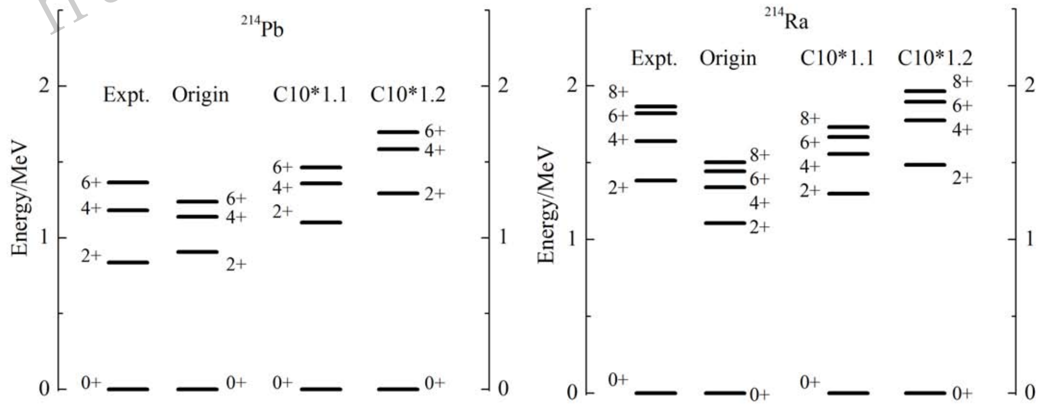

Fig. 1 Observed and theoretical levels of ^{214}Pb and ^{214}Ra where C10 is the T,S=1,0 channel of the central force in $V_{\rm MU}$. $V_{\rm MU}$. Observed levels are from Ref. [37].

Nuclei around ^{132}Sn and ^{208}Pb are selected to further examine the solidity of such "Mirror difference" effect and constrain the strength and its uncertainty of the central force, which are 105 levels in $^{125-130,134,136,138}$Sn and $^{201-206,210-212,214}$Pb and 83 levels in N=82 isotones with A=128,130,134∼139 and N=126 isotones with A=204∼206, 210∼214. It is shown in Fig. 2 that all these levels are described with an uncertainty around 0.2 MeV root mean square (RMS) when the strengths of the C10 and C11 channels are 105% and 100% of their original values, respectively.

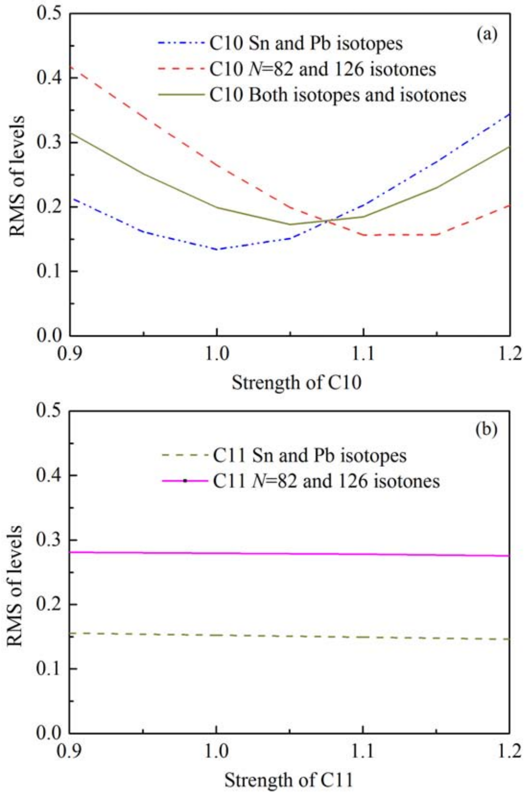

Fig. 2 (color online) Root mean square (RMS) between observed and theoretical levels as the function of the strength of the C10 (T,S=1,0) and C11 channels (T,S=1,1) of the central force in $V_{\rm MU}$. The levels are from Ref. [37] and selected from 105 levels in $^{125-130,134,136,138}$Sn and $^{201-206,210-212,214}$Pb and 83 levels in N=82 isotones with A=128,130, 134~139 and N=126 isotones with A=204~206, 210~214.

However, different minimums of RMS are found when the levels in these isotopes and isotones are separately considered, which means the strength of the pp interactions is around 15% larger than that of the nn interactions in ^{132}Sn and ^{208}Pb regions. Such "Mirror difference" may come from the renormalization effect of the bare nuclear force, because the protons and neutrons locate in different major shells. But more investigations are demanded to further and systematically understand this phenomena. Unlike the C10 channel, the C11 channel of the central force has almost no effect on the low-lying levels in ^{132}Sn and ^{208}Pb regions, as shown in Fig. 2. It is of great interesting to seek the levels, which are sensitive to the C11 channel.

After obtaining the effect of C10 channel on these levels, a simple statistical method, bootstrap method, can be used to obtain the uncertainty of the strength of C10 channel. 188 (105 or 83) levels are randomly selected from 188 (105 or 83) levels of Pb and Sn isotopes, and N=126 and 82 isotones (Pb and Sn isotopes only or N=126 and 82 isotones only). Because some levels may be selected more than one times and some may not be selected in a random selection, each time of random selection introduces a new sample and can be used to find the best parameter of C10 channel for this sample. After a million times of random selections, for samples selected from all levels, levels in isotopes only, and levels in isotones only, the mean values (standard deviations) of the strength of C10 channel are 105.2 (0.9)%, 100.1 (0.8)%, and 112.4 (2.5)% of the original value, respectively. It is clearly seen that the mean values are quite different, if levels in these isotopes and isotones are separately considered. It should be also noted that the present calculations have a sparse lattice on the strength of C10 channel, which is 5 MeV and should be further reduced to obtain a more reasonable evaluation on the mean values and standard deviations.

4 Cross-shell excitations in F isotopes

Three Hamiltonians, SDPF-M[34], SDPF-MU[27], and SDPF-USI[35], are used to investigate the cross-shell excitations in neutron-rich F isotopes. From Fig. 3, it is found that three Hamiltonians provide quite different descriptions on two neutron separation energies of F isotopes, especially when approaching to

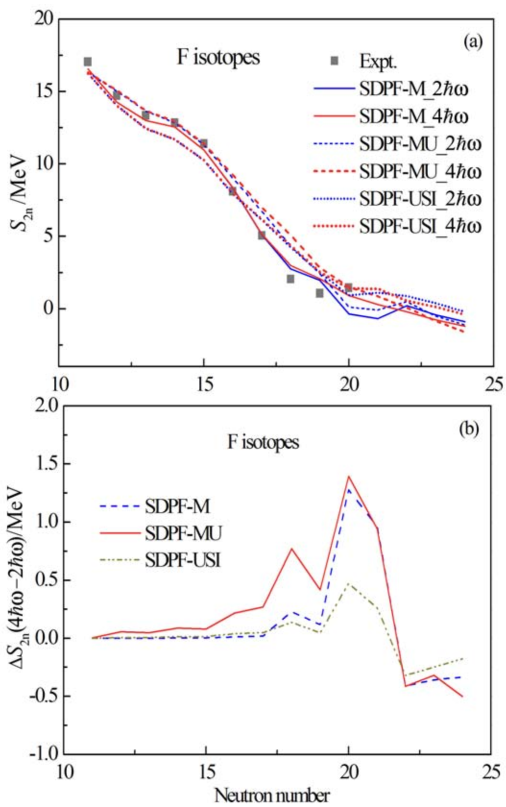

Fig. 3 (color online) Top: Observed and theoretical two neutron separation energies of neutron-rich F isotopes. Observed data are from Ref. [38]. Bottom: Differences between 4 and 2 $\hbar\omega$ calculations on two neutron separation energies.

N=20 shell gap. Despite the differences among three Hamiltonians, similar effect is found from the cross-shell excitations. The inclusion of the 4 $\hbar\omega$ configura tions provides additional bindings from results of all three Hamiltonians in F isotopes around N=20.

As shown in Fig. 3, the differences between 4 and 2$\hbar\omega$ results on two neutron separation energies of ^{29}F are around 1.4, 1.5, and 0.4 MeV in SDPF-M, SDPF-MU, and SDPF-USI, which means SDPF-USI gives a larger N=20 shell gap than SDPF-M and SDPF-MU. Because the location of the neutron drip line depends on the (two) neutron separation energies, the theoretical predictions on the neutron drip line are quite sensitive to the cross-shell configurations and interactions. It is worth to further investigate the single neutron spectrum inside and outside doubly magic nucleus on the drip line, ^{24}O, which can be used to constrain the calculations around ^{29}F. Because the present investigation starts from ^{16}O, which is too far from ^{29}F. If the monopole interaction is not exactly known, the single particle energies may not be well described far from ^{16}O.

The $5/2^+$ ground states and $1/2^+$ low-lying states in odd-even F isotopes are contributed by the single proton in *sd* shell. But as shown in Fig. 4, the calculated position of the $1/2^+$ state in ^{29}F is quite sensitive to the cross-shell excitations, which are expected to be dominated by the neutron excitations. The position of

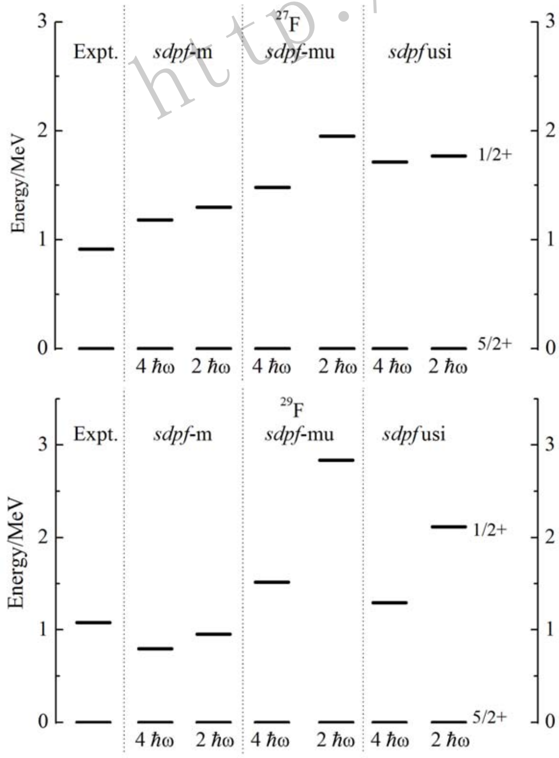

Fig. 4 Observed and theoretical levels of ^{27,29}F. Observed levels are from Ref. [37].

the $1/2^+$ states in F isotopes are useful to constrain both the *sd* shell and cross shell *pn* interaction, and the role of each part of the nuclear force, especially the tensor force.

Both Fig. 3 and Fig. 4 indicate the importance of the inclusion of the 4 $\hbar\omega$ configurations in F isotopes around ^{29}F, which means the cross-shell excitations are dominant configurations in these isotopes. If the 0 $\hbar\omega$ configurations are dominant, the impact of the 4 $\hbar\omega$ configurations is weak because the two-body interaction does not connect the 0 $\hbar\omega$ and 4 $\hbar\omega$ configurations. But if the 2 $\hbar\omega$ configurations are dominant, the contribution from 4 $\hbar\omega$ configurations is quite important. Certain deviations are found among three Hamiltonians, it is of great significance to investigate which part of the interaction contribute to these differences, such as the diagonal and the off-diagonal parts of the cross-shell excitations. The off-diagonal cross-shell interaction is shown to be very important to reproduce the levels and transitions in ^{14}C[33].

5 Conclusions

In summary, the present work provides preliminary investigations on the uncertainty of the central force and the effect of cross-shell excitations in the shell model. The 188 levels in semi-magic nuclei, Pb and Sn isotopes and N=82 and 126 isotones, are well described by a simple nuclear force V_{MU} + LS(M3Y). If the levels in these isotopes and isotones are separately considered, the root mean square (RMS) can be further reduced. The results show two different minimums of RMS for the C10 (T,S=1,0) channel of the central force in *pp* and *nn* interactions, while the strength of the former is around 15% stronger than that of the latter. The C11 (T,S=1,1) channel of the central force has almost no effect on the low-lying levels of these nuclei. The effect of cross-shell excitations are investigated on the two neutron separation energies and levels in neutron-rich F isotopes. Both of the properties around N=20 are strongly affected by the inclusion of the 4$\hbar\omega$ cross-shell excitations.

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壳模型中中心力不确定度和跨壳激发效应的初步研究

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摘要： 原子核壳模型不确定度虽然很重要，但目前为止还研究较少。本工作对壳模型中的核力不确定度和模型空间效应的展开了初步研究。核力中最重要的部分是中心力，中心力也被认为包含了最多的重整化效应。如果考虑半满壳核以及只考虑中心力的强度变化，对能谱的理论描述的变化只与中心力的C10(T,S=1,0)和C11(T,S=1,1) 部分相关。中心力变化时，自旋轨道耦合力和张量力都保持裸核力的强度不变。由此得到的简单核力的一套强度参数可以对Sn和Pb同位素及N=82和126同中素的188个态的能谱描述达到0.2 MeV均方根差。但是如果对这些同位素和同中素分别考虑，均方根差可以进一步减小，并且有不同的极小值。质子质子相互作用的强度比中子中子相互作用的强度要大15%，这表明中重核中存在“镜像能差”。增大模型空间对部分核的描述很重要，比如考虑跨壳激发对质子或中子数为幻数的核很重要。还通过三个哈密顿量研究了丰中子F同位素，尽管三个哈密顿量的结果不同，双中子分离能和能谱都对跨壳激发非常敏感，并且被跨壳激发影响的趋势类似。

关键词： 壳模型；不确定度；中心力；跨壳激发

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