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SHELL MODEL DESCRIPTION OF HEAVY NUCLEI AND ABNORMAL COLLECTIVE MOTIONS

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Abstract

I present briefly our systematic calculations on the spectroscopy and transition properties of intermediate-mass and heavy nuclei around ^{100}Sn and ^{208}Pb with realistic interactions, by using the large-scale configuration interaction shell model approach. I will show that the yrast spectra of Te isotopes present a vibrational-like equally spaced pattern, but the few known E2 transitions exhibit anomalous rotational-like behavior which cannot be reproduced by collective models. Moreover, the calculated B(E2) values for neutron-deficient and heavier Te isotopes show contrasting different behaviors along the yrast line, which may be related to the enhanced neutron-proton correlation when approaching $N = 50$. I will also take Pb isotopes as example to illustrate the application of the importance-truncation approach constructed based on the monopole Hamiltonian. For those nuclei, the full shell-model results also agree well with our generalized seniority and nucleon-pair-approximation truncation calculations. The deviations between theory and experiment concerning the excitation energies and electromagnetic properties of low-lying 0^+ and 2^+ excited states and isomeric states may provide a constraint on our understanding of nuclear deformation and intruder configuration in that region.

keywords: Configuration interaction shell model, intermediate-mass nuclei, E2 transition

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1 Introduction

The advent of radioactive ion beam facilities and new detector technologies has opened up new possibilities to investigate radioactive decays, structure and reaction properties of highly unstable nuclei [1]. These studies are now of particular importance in relation to the recent LIGO/VIRGO gravitational waves discovery and combined gamma-ray observations of the GW170817 neutron star merger. Recent investments in new or upgraded facilities such as FAIR at GSI, Darmstadt and FRIB at MSU will produce unprecedented data on exotic nuclei and nuclear matter that are relevant for neutron star mergers and the possible accompanying rapid neutron capture process. Moreover, one also aims at addressing fundamental nuclear physics questions including: How are complex nuclei built from their basic constituents and how can one explain collective phenomena from individual particle motion? In this contribution I would like to briefly discuss structure studies of intermediate-mass and heavy nuclei by using the so-called large-scale configuration interaction shell model approach. In particular, I will show its application in nuclei around ^{100}Sn and ^{208}Pb. Even though most of the nuclei mentioned below are on the neutron-deficient side, they are of interest since they are the longest isotopic chains that can be studied by the nuclear shell model and provide excellent background to study the competition of single-particle and two-body excitations.

Nuclear theory plays a critical role in explaining the regular emerging phenomena in nuclear many-body systems. The guiding principle for microscopic nuclear theory is that the building blocks of the nucleus, protons and neutrons, can be approximately treated as independent particles moving in a mean field that represents the average interaction between all particles. On top of that, one has to consider the residual interaction between different particles. The residual interaction depends on the choice of the mean field. It should be weak in the ideal case. The so-called *ab initio* approaches (in the sense that realistic nucleon-nucleon interactions are applied without significant *ad hoc* adjustment), the nuclear shell model defined in a finite model space and the density functional theory are among the most commonly employed nuclear models that have been developed. They treat the mean field in quite different ways. Within the *ab initio* family, the no-core shell model approach aims at considering the residual correlation between all nuclei in a large space defined by the harmonic oscillator single-particle orbitals. Those studies are constrained to very light nuclei. The nuclear shell model, as we call it, is a full configuration interaction approach. It considers the mixing effect of all possible configurations within a given model space. The model space is usually defined by taking a few single-particle orbitals near the Fermi surface. The number of orbitals one can include is highly restricted due to computational limitations. It may be useful to point out here that, in contrary to the first impressions of most people, the nuclear shell model calculation can be actually more challenging than many *ab initio* models from a computational point of view. Extenstive studies on algorithm optimization

and possible truncation or approximation methods have been carried out. State-of-the-art configuration interaction algorithms are able to diagonalize matrices with dimension up to 2×10^{10}. Other challenges of the no core and full configuration interaction shell model approaches include for examples the connection of their effective interaction to fundamental forces like the tensor force and three-body forces, and the complexity of the their wave function. Despite these challenges, the nuclear shell model is by far the most accurate and precise theory available on the market.

Below I will give a brief review on the challenges and recent developments of the nuclear configuration interaction shell model approach at our group. I will also mention a few simple but efficient truncation schemes. Shell-model calculations have been shown to be very successful in describing nuclei below ^{100}Sn. Now we aim at giving a microscopic description of heavier nuclei. I will show some results we obtained for intermediate-mass and heavy nuclei around ^{100}Sn and ^{208}Pb. I will explain the structure and decay studies of those nuclei, regarding both experimental and theoretical opportunities. A proper description of the $N = 126$ isotones is important for our understanding of the astrophysical r process and the possible existence of its third peak.

2 The shell model and selected applications

The residual interaction between valence particles around the Fermi surface is mostly supposed to be of a two-body nature. If the residual three-body interaction is neglected, the effective Hamiltonian in terms of single-particle energies and two-body matrix elements can be written as

$$H_{eff} = \sum_{\alpha} \varepsilon_{\alpha} \hat{N}_{\alpha} + \frac{1}{4} \sum_{\alpha\beta\delta\gamma JT} \langle \alpha\beta|V|\gamma\delta\rangle_{JT} A^{\dagger}_{JT;\alpha\beta} A_{JT;\delta\gamma}, \tag{2.1}$$

where we have assumed that the effective Hamiltonian conserves isospin symmetry, $\alpha = \{nlJT\}$ denote the single-particle orbitals and ε_{α} stand for the corresponding single-particle energies. $\hat{N}_{\alpha} = \sum_{j_z,t_z} a^{\dagger}_{\alpha,j_z,t_z} a_{\alpha,j_z,t_z}$ is the particle number operator. $\langle \alpha\beta|V|\gamma\delta\rangle_{JT}$ are the two-body matrix elements coupled to spin J and isospin T. A_{JT} ($A^{\dagger}_{JT}$) is the fermion pair annihilation (creation) operator.

One may rewrite the Hamiltonian as $H_{eff} = H_m + H_M$ where H_m and H_M denote the so-called monopole and Multipole Hamiltonians, respectively. The shell model energies can be written as

$$E_i^{\rm SM} = \sum_{\alpha} \varepsilon_{\alpha} < \hat{N}_{\alpha} > + \sum_{\alpha \le \beta} V_{m;\alpha\beta} \left\langle \frac{\hat{N}_{\alpha}(\hat{N}_{\beta} - \delta_{\alpha\beta})}{1 + \delta_{\alpha\beta}} \right\rangle + \langle \Psi_i | H_M | \Psi_i \rangle,$$

where $\sum_{\alpha} < \hat{N}_{\alpha} >= N$, Ψ_i is the calculated shell-model wave function of the state i. One often argues for the importance of the $T = 0$ monopole interaction in relation

to the fact that the $T = 0$ ones are mostly strongly attractive while the $T = 1$ ones are close to zero. However, it is the relative values among different $T = 0$ (or $T = 1$) channels that determines its relative importance. The relative value of the $T = 0$ and $T = 1$ monopole interaction $V_{0,1}$ only determines the relative position of the nuclear states with different total isospin T. The wave function is not necessarily changed.

Truncations often have to be applied in order to reduce the size of the shell-model bases. The simplest way of truncation is to restrict the maximal/minimal numbers of particles in different orbitals. This method is applied both to no-core (often being referred to Nmax) and empirical shell model (npnh) calculations. In Ref. [4] we studied the structure and electromagnetic transition properties of light Sn isotopes within the large $gdsh_{11/2}$ model space by restricting the maximal number of four neutrons that can be excited out of the $g_{9/2}$ orbital. However, the convergence can be very slow if there is no clear shell or subshell closure or if single-particle structure are significantly modified by the monopole interaction, as happens in neutron-rich light nuclei (see, e.g., Ref. [43]).

One can evaluate the importance of a given basis vector ψ_i within a partition through a perturbation measure $R_i = |\langle\psi_i|H_{eff}|\psi_c\rangle|/(\epsilon_i - \epsilon_c)$, where ψ_c is the chosen reference with unperturbed energy ϵ_c. It is expected that the basis vectors with larger R_i should play a larger role in the given state dominated by the reference basis ψ_c, from which a truncation scheme can be defined. The off-diagonal matrix elements $\langle\psi_i|H_{eff}|\psi_c\rangle$ are relatively weak in comparison to the diagonal ones. The most important configurations may be selected by considering the difference of unperturbed energy difference as $r_i = \epsilon_i - \epsilon_c$. A truncated model space can thus be defined by taking those states with smallest r_i. The challenge here is that the truncated basis may not conserve angular momentum. An angular momentum conserved correlated basis truncation approach is introduced in Ref. [20]. We are implementing this method in the widely distributed shell-model code NuShellX by replacing its projection subroutine with our new correlated basis method.

2.1 Nuclei around ^{100}Sn

The two-body matrix elements of the effective Hamiltonian can be calculated from realistic nucleon-nucleon potentials where one has to consider the effect of its short range repulsion and the core polarization effects induced by the assumed inert core. However, an optimization of the monopole interaction is necessary in most cases due to neglecting explicit three-body forces and other effects. The neutron single-particle states $d_{5/2}$ and $g_{7/2}$ orbitals in ^{101}Sn are expected to be very close to each other. A flip between the $g_{7/2}$ and $d_{5/2}$ orbitals from ^{103}Sn to ^{101}Sn was suggested in Ref. [9]. That result was used in the construction of the effective Hamiltonian [36] where the monopole interaction was optimized by fitting to all low-lying states in Sn isotopes using a global optimization method. The effective interaction has been shown to be successful in explaining many properties of nuclei in this region. We have been

evaluating the structure and decay properties of nuclei around $N = Z = 50$ and $Z = 82$ as well as heavier open-shell nuclei within $gdsh_{11/2}$ shell (see, for examples, Refs. [39, 40]).

It was argued that ^{100}Sn may be a soft core in analogy to the soft $N = Z = 28$ core ^{56}Ni. It seems such a possibility can be ruled out based on indirect information from recent measurements in this region [3, 4, 13, 15, 17]. The asymmetric electric quadrupole (E2) transition shape in Sn isotopes is suggested to be induced by the Pauli blocking effect [4]. A systematic study on the E2 transition in Te isotopes is done in Ref. [13]. One can state that the limited number of valence protons and neutrons are not expected to induce any significant quadrupole correlation in this region [5, 8, 16, 41].

For systems involving the same kind of particles, the low-lying states can be well described within the seniority scheme [38]. This is related to the fact that the $T = 1$ two-body matrix element is dominated by $J = 0$ pairing interactions. The seniority number is related to the number of particles that are not paired to $J = 0$. Our recent studies on the seniority coupling scheme may be found in Refs. [18, 24, 28, 29, 32, 35]. One can also derive the exact solution of the pairing Hamiltonian by diagolizing the matrix spanned by the seniority $v = 0$, spin $I = 0$ states which represent only a tiny part of the total wave function. This is applied in Ref. [7, 33, 43]. The seniority coupling can be broken if both protons and neutrons are present where neutron-proton (np) coupling may be favored. In relation to that, there has been a long quest for the possible existence of np pairing in $N \sim Z$ nuclei (see, recent discussions in Refs. [6, 14, 26, 27, 42]). We have also done pair-truncated shell-model calculations with collective pairs as building blocks in Refs. [19, 34, 42] for both the standard shell model and continuum shell model in the complex energy plane. One example is the proton-unbound nucleus ^{109}I [22] for which the level structure and E2 transition properties are very similar to those of ^{108}Te [3] and ^{109}Te [23], indicating that the odd proton in ^{109}I is weakly coupled to the ^{108}Te daughter nucleus, like a spectator.

The low-lying collective excitations of mid-shell Cd and Te isotopes were discussed in terms of quadrupole vibrations [11, 16] in relation to the fact that the even-even isotopes between $N = 56$ and 70 show regular equally-spaced yrast spectra. If that is the case, those isotopes will provide an ideal ground to explore the nature of the elusive nuclear vibration. However, the available E2 transition strengths along the yrast line in $^{114,120-124}$Te show an anomalous rotational-like behavior [21,37]. It can not be reproduced by collective models or the interacting boson model. Another intriguing phenomenon is the nearly constant behavior of the energies of the 2^+ and 4^+ states in Te and Xe isotopes and their ratios when approaching $N = 50$, in contrast to the decreasing behavior when approaching $N = 82$ [16]. This was analyzed in Ref. [10] based on the quasiparticle random phase approximation approach. We have done systematic calculations on the E2 transition properties of Te isotopes in Ref. [31]. The calculations reproduce well the excitation energies of

the low-lying states as well as the regular and vibrational-like behavior of the yrast spectra of $^{108-130}$Te. In particular, the calculations reproduced reasonably well the nearly constant behavior of the $B(E2)$ values of ^{114}Te and $^{120-124}$Te along the yrast line. The anomalous constant behavior is related to the competition between the seniority coupling and the neutron-proton correlations. On the other hand, a squeezed gap between the 6_1^+ and 4_1^+ states is seen in Te isotopes when approaching $N = 82$, resulting in seniority-like spectra. A further experiment is done to study the angular momentum dependence of the E2 transition strengths in ^{112}Te [12]. It shows a similar but more 'vibrational'-like behavior. Potential-Energy Surface calcultions indicate that those nuclei may also be understood from a soft rotor point of view.

Further calculations on the E2 transitions of Cd isotopes (with two proton holes instead of particles within $Z = 50$ closure) are underway.

2.2 Pb isotopes

We have done a systematic calculation on the structure and electromagnetic transition properties of neutron-deficient PB isotopes, which may be studided experimentally using the AGATA detector. Our shell-model calculations can reproduce well the excitation energies of the low-lying 0^+ and 2^+ states in isotopes $^{198-206}$Pb [34]. The overall agreement between experiments and calculations are quite satisfactory. For nuclei heavier than ^{196}Pb, the difference between theory and experiment is less than 100 keV. The largest deviation appears in the case of ^{194}Pb for which the calculation overestimates E^{SM} by 300 keV. The empirical pairing gaps can be extracted from the binding energy by using the simple three-point formula. They carry important information on the two-nucleon pair clustering as well as α clustering in the nuclei involved [2, 25]. In nuclear systems, the pairing collectivity manifests itself through the coherent contribution of many shell-model configurations, which lead to large pairing gaps.

The excitation energies of the first 2^+ isotopes in Pb isotopes show a rather weak parabolic behavior. In the lighter Pb isotopes, the excitation energy of the second 0^+ state decreases rapidly with decreasing neutron number. It even becomes the first excited state in $^{184-194}$Pb. Within a shell-model context, those low-lying 0^+ states may be interpreted as coexisting deformed states which are induced by proton pair excitations across the $Z = 82$ shell gap. The energy of those core-excited configurations becomes more favored in mid-shell Pb isotopes, in relation to the stronger neutron-proton correlation in those nuclei.

We have developed an importance truncation based on the total monopole energy as [34]

$$E_P^{\rm m} = \sum_\alpha \varepsilon_\alpha N_{P;\alpha} + \sum_{\alpha\le\beta} V_{m;\alpha\beta} \frac{N_{P;\alpha}(N_{P;\beta} - \delta_{\alpha\beta})}{1+\delta_{\alpha\beta}}, \tag{3.1}$$

where $N_{P;\alpha}$ denotes the particle distributions within a given partition P. One can order all partitions according to the monopole energy $E_P^{\rm m}$ and consider the lowest

ones for a given truncation calculation. The idea behind is that the Hamiltonian is dominated by the diagonal monopole channel. The monopole interaction can change significantly the (effective) mean field and drive the evolution of the shell structure. We have done truncation calculations for two isotopes ^{200,194}Pb. Convergence can be reached with a small portion (around 10%) of the total M-scheme wave function in both cases. This truncation approach can be easily implemented in most existing shell model codes [30].

3 Summary and future work

I presented briefly our recent work on the configuration interaction shell model calculations of the spectroscopy and transition properties of intermediate-mass and heavy nuclei. I started by introducing the basic framework of the nuclear shell model and the monople channel of the effective Hamiltonian. A simple truncation scheme can be established by considering configurations with lowest monopole energies, which I refer to as the importance-truncation approach. Good convergence for Pb isotopes is reached from both the energy and wave function perspectives. Large scale calculations are carried out to study the spectroscopic and transition properties of nuclei around ^{100}Sn and ^{208}Pb that cannot be reached by standard shell model calculations.

Our effective Hamiltonians have been globally optimized for describing the Sn and Pb isotopes, which work well also for most open-shell nuclei. As an example, I mentioned the Te isotopes. The yrast spectra of Te isotopes show a vibrational-like equally spaced pattern, but the few known E2 transitions show anomalous rotational-like behahavior which cannot be reproduced by collective models. Moreover, the calculated B(E2) values for neutron-deficient and heavier Te isotopes show contrasting different behaviors along the yrast line, which may be related to the enhanced neutron-proton correlation when approaching $N = 50$. The Hamiltonian works well also for Sb, I and Xe isotopes but shows relatively larger deviations from experimental data for selected other nuclei including Cs and Lu isotopes. An analysis of the origin of the deviations is underway. We are also optimzing the $T = 0$ channel of the effective interaction. In addition, we are extending the model space to include orbitals between the $N = Z = 50$ shell closure as well as neutron orbitals above $N = 82$ in order to study the structure of neutron-rich Cd isotopes.

For Pb isotopes, the full shell-model results also agree well with our generalized seniority and nucleon-pair-approximation truncation calculations. The deviations between theory and experiment concerning the excitation energies and electromagnetic properties of low-lying 0^+ and 2^+ excited and isomeric states indicate that, as suggested by deformed mean field calculations, nuclear deformation as an induced intruder configuration from outside the model space should be important for nuclei in that region. Large-scale calculations are being carried out by including by neutron and proton core excited configuration.

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