Large-Scale Shell Model Calculations of Heavy Nuclei

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Abstract

In this contribution I describe briefly the application of the shell model configuration interaction approach to intermediate-mass and heavy nuclei at KTH. I focus in particular on the technical side of the development which enables us not only to perform large-scale full-configuration interaction calculations but also to solve efficiently the nuclear pairing Hamiltonian in a truncated space defined by seniority.

Keywords: *Nuclear shell model; truncation; pairing; collective motion*

1 Introduction

In the talk I present systematic calculations of the spectroscopy and transition properties of intermediate-mass and heavy nuclei around doubly magic ^{100}Sn as well as around ^{208}Pb by using the large-scale configuration interaction shell model approach with realistic interactions. Those nuclei are of interest to us partially due to the fact that they are the longest isotopic chains that can be studied by the nuclear shell model. We hope they can provide excellent background to study the competition of single-particle and two-body excitations. In particular, we studied the yrast spectra of Te isotopes which show a vibrational-like equally-spaced pattern but a few known $E2$ transitions show anomalous rotational-like behaviour, which cannot be reproduced by collective models [1–6]. Moreover, the calculated $B(E2)$ values for neutron-deficient and heavier Te isotopes show contrasting different behaviours along the yrast line. This may be related to the enhanced neutron-proton correlation when approaching $N = 50$. In general, 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 interaction and a hint on possible quantum phase transition. We have measured the lifetimes of the first excited 2^+ and 4^+ states in the neutron-deficient nuclide ^{172}Pt [7]. We have also done several large-scale shell model calculations with realistic nucleon-nucleon interactions for Pt, Os and W isotopes between $N = 82$ and 94 by considering either ^{132}Sn or ^{146}Gd as the inert cores. A striking feature we found is that the ratio $B(E2; 4_1^+ \rightarrow 2_1^+)/B(E2; 2_1^+ \rightarrow g.s.) = 0.55(19)$ is unusually low. In

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http://www.ntse.khb.ru/files/uploads/2018/proceedings/Qi.pdf.

addition, a few other neutron-deficient W, Os, and Pt nuclei in this region feature the same effect [8].

In this talk I also illustrate the application of the importance-truncation approach, which is based on the monopole Hamiltonian, to neutron deficient Pb isotopes [9]. For those nuclei, the full shell-model results also agree well with our generalized seniority and nucleon-pair-approximation truncation calculations. We have developed an angular momentum projection technique to derive the analytic wave functions and energy expressions for those states in the simplified single-j case [10].

In this Proceeding, I would like to focus on some technical details of our efforts at KTH, Stockholm in developing the shell model algorithm and its possible various applications. In addition to large-scale full and truncated configuration interaction calculations, one of our primary interests is to apply the model to solve the pairing Hamiltonian in large model space efficiently.

2 Shell model approach

The shell model we refer to, deals with residual interaction between valence particles around the Fermi surface, which is mostly supposed to be of a two-body nature. The effective Hamiltonians in terms of single-particle energies and two-body matrix elements can be written as follows,

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

where we assume that the effective Hamiltonian conserves isospin symmetry, $\alpha = \{nljt\}$ denotes the single-particle orbitals and ε_{α} stands 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.

The pairing matrix elements refer to those with $J = 0$ and α and β (as well as δ and γ) corresponding to time reversal orbitals. One has

$$H_P = \sum_{\alpha} \varepsilon_{\alpha}\, \hat{N}_{\alpha} + \frac{1}{4} \sum_{\alpha\overline{\alpha}\gamma\overline{\gamma}T} \langle \alpha\overline{\alpha}|V|\gamma\overline{\gamma}\rangle_{J=0T}\, A^{\dagger}_{JT;\alpha\overline{\alpha}}\, A_{JT;\gamma\overline{\gamma}}. \tag{2}$$

In most mean field approaches, usually the proton-proton and neutron-neutron pairing are considered only. The neutron and proton pair can couple to both $T = 1$ (isovector) and $T = 0$ (isoscalar). The importance of neutron-proton correlation may also become important in $N \sim Z$ nuclei. In relation to that, there is a long-standing quest for a possible existence of the np pairing in $N \sim Z$ nuclei (see recent discussions in Refs. [11–15]).

The monopole Hamiltonian determines average energy of eigenstates in a given configuration. The monopole interaction itself does not induce any mixture between different configurations, however it can change significantly the (effective) mean field and drive the evolution of the shell structure. The monopole interaction V_m is the angular momentum averaged effects of the two-body interaction,

$$V_{m,\alpha\beta} = \frac{\sum_J (2J+1)\, V^J_{\alpha\beta\alpha\beta}}{\sum_J (2J+1)[1-\delta_{\alpha\beta}(-1)^J]} = \frac{\sum_J (2J+1) V^J_{\alpha\beta\alpha\beta}}{(2j_{\alpha}+1)} \frac{1+\delta_{\alpha\beta}}{2j_{\beta}+1-\delta_{\alpha\beta}}. \tag{3}$$

The strong mixture of the wave function is mainly induced by the residual $J = 0$ pairing and the QQ neutron-proton interaction in the multipole Hamiltonian. However, a tricky issue one often get confused is that the diagonal matrix elements of the pairing Hamiltonian (with $\alpha = \gamma$) also contribute significantly to the monopole interaction.

The number of orbitals one can include is strongly restricted due to the computational limitation. Extensive studies of the algorithm optimizations and possible truncation or approximation methods have been carried out. State-of-the-art configuration interaction algorithms are able to diagonalize matrices with dimensions up to 2×10^{10} with the shell model codes like KSHELL and Redstick. Truncations often have to be applied in order to reduce the sizes of the shell-model bases. The simplest way of the truncation is to restrict the maximal/minimal numbers of particles in different orbitals. This method is applied to both the no-core (often being referred to as $N_{\max}$) and empirical shell model (np–nh) calculations. We studied in Ref. [1] the structure and electromagnetic transition properties of light Sn isotopes within the large $gdsh_{11/2}$ model space by restricting to four the maximal number of 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 the single-particle structure is significantly modified by the monopole interaction, as it happens in neutron-rich light nuclei (see, e. g., Ref. [16]).

One can evaluate the importance of a given basis vector ψ_i within a partition through the perturbation measure $R_i = |\langle\psi_i|H_{eff}|\psi_c\rangle|/(\epsilon_i - \epsilon_c)$ where ψ_c is the chosen reference state with the unperturbed energy ϵ_c. It is expected that the basis vectors with larger R_i should play larger role in the given state dominated by the reference basis state ψ_c used to define the truncation scheme. 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 unperturbed energy difference $r_i = \epsilon_i - \epsilon_c$. A truncated model space can thus be defined by taking the vectors with smallest r_i. The challenge here is that the truncated bases may not conserve angular momentum. An angular momentum conserved correlated basis truncation approach was introduced in Ref. [17]. We are implementing this method in the widely distributed shell-model code NuShellX by replacing its projection subroutine with our new correlated basis method.

An importance truncation can be introduced based on the total monopole energy by considering the multipole Hamiltonian as a perturbation. The idea behind is again that the Hamiltonian is dominated by the diagonal monopole channel. One can evaluate the total monopole energy of a given partition $\mathcal{P}$ as

$$E^{\mathrm{m}}_{\mathcal{P}} = \sum_{\alpha} \varepsilon_{\alpha} N_{\mathcal{P};\alpha} + \sum_{\alpha \leq \beta} V_{m;\alpha\beta} \frac{N_{\mathcal{P};\alpha}(N_{\mathcal{P};\beta} - \delta_{\alpha\beta})}{1 + \delta_{\alpha\beta}}, \tag{4}$$

where $N_{\mathcal{P};\alpha}$ denotes the particle distributions within a given partition $\mathcal{P}$. One can order all partitions according to the monopole energy $E^{\mathrm{m}}_{\mathcal{P}}$ and consider the lowest ones for a given truncation calculation. Moreover, it is expected that the pairing correlation should play a significant role governing the structure of the lowest-lying states of the semi-magic Pb isotopes. This model was applied in our calculations of Pb isotopes [9]. Convergence is mostly achieved at $d/D \sim 0.1$, i. e., by considering only 10% of the total M-scheme bases. This method is very easy to implement and it preserves the simplicity of the M-scheme algorithm.

We have also done pair-truncated shell-model calculations with collective pairs as building blocks in Refs. [9, 14, 18] for both the standard shell model and continuum shell model in the complex energy plane.

3 Exact diagonalization of pairing Hamiltonian

The pairing Hamiltonian is usually solved using the simple BCS or the HFB approach which both violate the conservation of the number of particles. Particle-number-conserved pairing calculations can be done within the Richardson approach (see, e. g., Ref. [19]) or utilizing the exact diagonalization in a way similar to the shell model [16, 20]. The Richardson approach can be applied to very large (infinite) systems but is limited to Hamiltonians of a certain form. On the other hand, the exact diagonalization can be done for a general Hamiltonian but the number of orbitals one can include is limited. This limitation makes is difficult to perform realistic calculations and to compare the results with those from the BCS or similar approaches. In addition, it limits the application of the model to the α decay or pair transfer reaction calculations. This is one of the challenges we have been trying to resolve in the past few years. We have developed a very efficient and robust solver for the Richardson equation which will be publicly available soon. We have also developed two large-scale exact diagonalizers: one is based on our large-scale shell model code and parallelized using MPI + OpenMP hybrid algorithm; the other one uses only OpenMP parallelization which can be easily combined with existing mean field codes to replace the problematic BCS solver.

We have developed a seniority truncation approach for the M-scheme shell model algorithms. For systems comprising the particles of the same kind, the low-lying states can be well described within the seniority scheme. This is related to the fact that the $T = 1$ two-body matrix elements are dominated by the $J = 0$ pairing interactions. The seniority is related to the number of particles that are not paired to $J = 0$. The seniority coupling has shown a remarkable success in describing the spectroscopy and electromagnetic transition properties of semi-magic nuclei with spherical symmetry. Our recent studies on the seniority coupling scheme may be found in Refs. [21–26]. The standard seniority coupling cannot be utilized within the M-scheme shell model code where the angular momentum conservation is not considered at the basis vector level. On the other hand, we can define a seniority-like M-scheme pair. We set this 'seniority' to zero if all particle pairs can be coupled to $M = 0$ that is all orbitals have their time reversal partners. The seniority in our M-scheme refers then to the number of particles that have no time reversal partners.

One can derive the exact solution of the pairing Hamiltonian by diagonalizing the matrix spanned by the seniority $v = 0$, spin $I = 0$ states which represent only a tiny part of the total wave function. Our second code is designed in such a way that it works only in the $v = 0$ or low seniority cases but in a very simple and efficient way. If only the seniority $v = 0$ states are considered, there is ONLY one basis vector for each shell model partition. This allows us to generate the $v = 0$ basis in a way similar to the M-scheme shell model. We take one time reversal orbital pair as one binary bit which is represented as '1' if the orbital is occupied. So, the combination problem of generating all possible M-scheme vectors with a fixed number of identical pairs N in M time reversal states is equal to generating binary integers consisting of the same N number of digit '1' and $M - N$ number of digit '0'. As an example,

for three pairs in six doubly degenerate orbitals, an obvious basis would be '000111' which is easy to generate and which has the minimum value. The basis with maximum value can also be generated simply. Then we have a two-step mechanism to generate the rest basis vectors: For an input binary integer, first, find the first two adjacent bits with the binary pattern '01' and turn them to '10'; second, move all digit '1' on the lower side of the turned '10' to the lowermost. The next larger integer is then generated. The iteration should start from the minimum as input and be stopped when the output is equal to the maximum.

We take again the above system as an example: the two-step mechanism starts from the vector 000111 with the minimum value; the first '01' appears at the third bit, we turn '01' to '10' and '000111' is turned to '001011'; since all digit '1' is on the lowermost, the output is '001011'. From this basis, we can generate '001101' and '001110'. For the basis '001110', we flip the first '01' which changes the basis to '010110'. However, on the lower side of the fourth bit, there are two digits '1' at the second and the third bit which should be moved to the lowermost, so the final output is '010011'. This simple mechanism allows us to generate a large-scale basis in a very efficient manner which was actually a bottleneck for us before.

A remarkable feature is that the algorithm works also in the case of degenerate systems which allow more than one pair in a single orbital. In such situations, we at first represent an orbital with degeneracy D as $D/2$ continuous bits. One can, of course, generate the basis in the same way as above. We have a complete M-scheme basis for which the solution will be eigenstates of the spherical pairing Hamiltonian. However, one should bear in mind that the dimension of such a M-scheme-like basis set can be orders of magnitude larger than the J-scheme-like seniority-zero basis which makes the calculations much less efficient.

To overcome this problem, we label the bits from the same degenerate orbital as a subgroup. Inside each subgroup, since all particles are indistinguishable, we just need one vector to represent different combination of bits, and the easiest choice is to put all digit '1' on the lowermost side. For example, '000111' can represent uniquely the vector for a system with three pairs in a 12-fold orbital. All the rest will be neglected. In other words, we will do not flip the '01' within a given subgroup.

The basis vectors generated with the above algorithm are ordered accordingly to their values. This also allows us to identify the non-zero Hamiltonian matrix elements in an efficient way. For a given vector $|\phi_i\rangle$ we first generate a subbasis set from the operation $\phi_j = H|\phi_i\rangle$. The indices of the subbasis ϕ_j can be determined then by matching their values with those from the original basis set using standard searching algorithms. It can be quite efficient since the basis vectors are ordered.

With the code described above, one can readily solve a half-filled system with up to 36–38 doubly-degenerate orbitals and 18–19 pairs (with dimensions 9×10^9–3.5×10^{10}). The corresponding shell-model space dimensions are around 4×10^{20}–7×10^{21}) which is a problem formidable to solve.

The code works efficiently on PC, and now we are combing the code with publicly available Hartree–Fock (HF) mean field codes for realistic calculations. One of our concerns is the contribution of the pairing matrix elements to the monopole energy.

Let us consider a simple system with N pairs of identical particles in a single-j shell. The total energy can be obtained as

$$E = N(N-1)G - N\Omega G, \tag{5}$$

where G is the pair coupling constant and $\Omega = j + 1/2$. The first linear term on the right hand side corresponds to the contribution of the pairing to the monopole channel or the mean field, and the second term defines the pairing correlation energy

$$E_{\rm corr} = N(N - \Omega)G. \tag{6}$$

This aspect looks simple but should be properly taken into account when the pairing Hamiltonian is solved exactly to evaluate the pairing correlation or to be compared with the BCS approach. For a system involving equally-spaced doubly-degenerate orbitals, we showed that the total energy can be also rather well approximated as [20]

$$E(N) \simeq N\,(N-1)\,\mathcal{G} + NE_2, \tag{7}$$

where $\mathcal{G}$ is a coefficient related to the pairing strength and level density. One has

$$\begin{aligned} E_{\rm corr}(N) &\simeq N\,(N-1)\,\mathcal{G} + NE_2 - N(N+1) + NG \\ &= N\,(N-1)\,(\mathcal{G}-1) + N(E_2 - 2 + G), \end{aligned} \tag{8}$$

where the first and the second terms define the Pauli blocking effect and the correlation energy of a single pair, respectively.

As discussed above, the diagonal channel of the full pairing Hamiltonian contributes significantly to the total binding energy, which may result in an over-counting problem and has to be removed from the exact solution of the pairing Hamiltonian in the mean field applications. In some cases, the diagonal matrix elements are removed in analogy to the BCS approach, and the following Hamiltonian is diagonalized,

$$H' = \sum_{\alpha} \varepsilon \hat{n}_{\alpha} - \sum_{\alpha \neq \beta} G_{\alpha\beta}\, a^{\dagger}_{\alpha} a^{\dagger}_{\bar{\alpha}} a_{\beta} a_{\bar{\beta}}, \tag{9}$$

where α runs again over the time-reversal orbits with quantum numbers j_α and $|m_\alpha|$ within the HF configuration. In this way one excludes the renormalization effect of the single-particle energy from the diagonal pairing matrix elements. The disadvantage is that the rotational symmetry is not conserved at the two-body level.

The *de facto* standard approach to extract the correlation energy is to take the difference between the total energy E and the energy of the lowest, unperturbed HF configuration as

$$E_{\rm corr} = E - E_{HF}, \tag{10}$$

where $E_{\rm corr}$ is the (negative) correlation energy and E_{HF} is the HF energy which provides the upper bound for the total energy and is the starting point for various post-HF calculations of the correlation. One can define in a straightforward way the correlation energy as

$$E^{(1)}_{\rm corr} = E_{gs} - \sum_{\alpha} [2\varepsilon_{\alpha} - G_{\alpha\alpha}], \tag{11}$$

where E_{gs} is the lowest energy. $G_{\alpha\alpha}$ are the corresponding diagonal matrix elements.

Now we introduce a different definition for the correlation energy based properly on the definition of the monopole interaction. If only the pairing interaction is considered for the particle-particle channel, we have $V^{J=0}_{jjjj} = -\Omega_j G_{jj}$ and $V_{jj} = -G_{jj}/2j$. Thus one can define an alternate way to calculate the correlation energy as

$$E^{(2)}_{\rm corr} = E - \sum_{j \in HF} \left[n_j \varepsilon_j - \frac{G_{jj}}{2j} \frac{n_j(n_j-1)}{2} \right], \tag{12}$$

where j runs over all single-j levels within the HF configuration.

$E^{(1)}_{\rm corr}$ and $E^{(2)}_{\rm corr}$ would be identical if all single-particle levels within the HF configuration are fully occupied. However, it should be emphasized that $E^{(2)}_{\rm corr}$ gives a stronger (negative) correlation energy than $E^{(1)}_{\rm corr}$ if the last orbital is only partially occupied (with $N = 1$ to $\Omega - 1$ pairs). The deviation is

$$E^{(2)}_{\rm corr} - E^{(1)}_{\rm corr} = -N_k(\Omega_k - N_k)\frac{G_{kk}}{\Omega_k - 1/2}, \tag{13}$$

where k corresponds to the last occupied orbital and $N_k(\Omega_k - N_k) = (\Omega_k u_k v_k)^2$. This deviation is related to the fundamental difference between the coupling of particles in the two schemes: The particles are constrained to pair to zero angular momentum with its time reversed partner in the former case but there is no such constraint in the second case. This is the reason why $E^{(2)}_{\rm corr}$ predicts more correlation energy than the first case. With the pairing correlation energy thus defined, we can perform now a systematic study of nuclear masses.

4 Summary

In this talk, I presented our recent works on the configuration-interaction shell-model calculations of the spectroscopy and transition properties of intermediate-mass and heavy nuclei. In this contribution to the Proceedings, I started by introducing the basic framework of the nuclear shell model and of the monopole channel of the effective Hamiltonian. A simple truncation scheme can be established by considering configurations with the lowest monopole energies, which I refer to as the importance-truncation approach. A seniority-like truncation has also been introduced, which allows to apply the large-scale shell model algorithm to the problem of solving the standard pairing Hamiltonians. We introduced a simple but efficient way to generate the basis for the paired states and for calculating the non-zero Hamiltonian matrix elements. We also discussed different ways to exclude the pairing contribution to the monopole interaction in order to utilize our thus developed exact pairing solver in realistic mean field calculations.

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