

Computational issues of configuration interaction frameworks describing open quantum systems

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Abstract. Open quantum systems (OQS), extended in space (halo nuclei) or even unbound, differ from closed quantum systems (CQS), for which the methods of standard shell model (SM) [1] can be utilized in order to expand their wave function in a configuration interaction framework. Configuration interaction methods based on the use of Berggren bases [2], comprising bound, resonant and scattering states, which have the ability to generate the very long range asymptotic behavior of OQSs, are used instead for that matter. This demands the introduction of new computational techniques, including the optimization and discretization of the Berggren basis [3], the development of an algorithm to efficiently calculate their two-body matrix elements [4], and an overall optimization of memory storage absent from SM, where, for instance, all data related to proton and neutron spaces only can be precalculated and stored [1]. In order to diagonalize the very large induced matrices, the Density Matrix Renormalization Group (DMRG) method [5] extended to OQSs has been developed [6, 7]. A renormalization procedure which generates more and more correlated many-body basis states iteratively is used therein, so that the Hamiltonian matrix to diagonalize is very small compared to that occurring with a many-body basis of independent particles [6, 7]. Parallelization of presented methods will also be discussed.

1. Introduction

The precise description of drip-line nuclei is a challenge for both theoretical and experimental nuclear physics. Along with the advent of radioactive beams provided by accelerators of new generation, it is now possible to synthesize very short-lived nuclei, bearing important neutron-to-proton ratio, whose study will provide new experimental data which will have to be explained at theoretical level. The most exotic nuclei, contrary to those situated in the valley of stability, exhibit special features originating from the proximity of proton or neutron emission threshold. One of the most interesting phenomenon is the appearance of halos, i.e. nuclei which are extended beyond classically allowed regions. Due to the strong coupling with the continuum of scattering states, nuclear correlations and continuum effects mix together and give rise to complex nuclear structures. One can also mention the existence of Borromean nuclei, for which all subsystems are unbound, but so that the whole system is bound because of the correlations between its subparts. While these properties exist in the vicinity of proton and neutron drip-lines, the proton drip-line itself has unique properties, such as two-proton radioactivity, discovered a few years ago [8]. Another peculiarity is the redistribution of shell closures close to drip-lines [9]. Considering the very different natures of the nuclei of the valley of stability and drip-lines, new theoretical models must be formulated in order to provide a uniform vision of the nuclear chart. For this, the



standard configuration interaction model of nuclear physics, called SM [1], must be extended. Indeed, SM is based on the use of the one-body harmonic oscillator basis, whose one-body states generate the many-body Slater determinant basis, upon which many-body nuclear states are expanded. Despite its numerous analytical advantages (analytical matrix elements, exact treatment of the center of mass motion, ...), the use of the harmonic oscillator basis is confined to the description of well-bound many-body states, as the necessary truncation of the many-body Slater determinant basis and the Gaussian fall-off of harmonic oscillator states implies that the asymptotic of many-body nuclear states is always falling very rapidly. Hence, far-extended states such as halo and resonant nuclear states cannot be described with this formalism. A solution to this problem is the use of the Gamow Shell Model (GSM) [10, 11, 12, 13, 14, 15, 16, 17]. GSM is an extension of the SM, where a basis of complex energy states, the Berggren basis [2], is used instead of a basis generated by a harmonic oscillator potential. The Berggren basis consists of bound, resonant (or Gamow states [18]), and of complex-energy scattering states. This model allows to expand A -body halo and resonant correlated nuclear states. Consequently, extended many-body asymptotic can be handled with the Berggren basis. However, due to the fact that it contains a continuous part, which must be discretized, the number of one-body states to consider in a numerical calculation becomes very large, so that the standard numerical techniques of many-body diagonalization, based on the Lanczos method, can no longer be used. Indeed, matrices to diagonalize become very much larger than in SM, whose current limit is around one billion and demands advanced numerical methods to be handled. In order to counter this state of affairs, the DMRG method [15] has been introduced, where the direct diagonalization of large matrices is replaced by an iterative construction of correlated basis states, whose number is sufficiently small so as to allow standard diagonalization techniques to be used. It is thus the object of this article to describe configuration interaction models using the Berggren basis on the hand, and to emphasize the numerical problems that it generates and how they are solved using parallel computation techniques on the other hand.

2. Berggren basis of one-body states

The standard completeness relation of Newton [19] is the decomposition of unity formed by the bound and real-energy scattering states generated by a finite-range potential:

$$\sum_{n \in b} u_n(r) u_n(r') + \int_0^{+\infty} u(k, r) u(k, r') dk = 1, \quad (1)$$

where $u_n(r)$ is a normalized bound state and $u(k, r)$ a scattering state of linear momentum k , normalized so that in the asymptotic region, where $u(k, r) = C_+ H_{\ell, \eta}^+(kr) + C_- H_{\ell, \eta}^-(kr)$ ($H_{\ell, \eta}^\pm$ is a Hankel or Coulomb wave function of orbital angular momentum ℓ and Sommerfeld parameter η), $2\pi C_+ C_- = 1$. This is equivalent to the normalization of scattering states to a Dirac delta. The completeness relation of (1) allows to expand integrable states. By deforming the real k -axis in the complex plane, thus enclosing narrow resonant states (see figure 1), which are poles of the S -matrix and are defined with outgoing wave function condition only ($C_- = 0$), Cauchy theorem implies that:

$$\sum_{n \in (b, d)} u_n(r) u_n(r') + \int_{L^+} u(k, r) u(k, r') dk = 1, \quad (2)$$

where $u_n(r)$ is at present a bound or decaying state lying between the real axis and the contour of complex linear momenta L^+ . This is the Berggren completeness relation, introduced for the first time in [2]. One can expand bound or resonant states with (2). Note that resonant states are unbound, so that they cannot be normalized on the real axis as bound states, as their norm

would diverge. To solve this problem, exterior complex scaling is utilized to define the norm of resonant states, where integration is effected on a contour of the complex plane where the resonant state decreases exponentially [20].

The completeness relations of Newton and Berggren have been demonstrated for potentials decreasing quickly on the real axis, i.e. for the neutron case in [2, 19], and they have been extended to the proton case, where the generating potential possesses an infinite-range Coulomb part, in [21]. In order to use the Berggren basis numerically, one has to discretize the continuum of complex-energy states. For this, the Gauss-Legendre quadrature is employed. Denoting (k_i, w_i) the N_c linear momenta discretized and their respective weight, (2) writes after discretization:

$$\sum_{n \in (b,d)} u_n(r)u_n(r') + \sum_{i=1}^{N_c} u(k_i, r)u(k_i, r') w_i \sim 1. \quad (3)$$

In order to render (3) formally identical to that of a discrete basis, as that generated by a harmonic oscillator potential, one redefines the complex-energy scattering states by $u_{i+N_d}(r) = u(k_i, r)\sqrt{w_i}$, where N_d is the number of discrete bound and resonant states. Hence, writing the bound and resonant states as $u_i(r) = u_n(r)$, where $i \leq N_d$, one obtains the requested formulation of (3):

$$\sum_{i=1}^N u_i(r)u_i(r') \sim 1, \quad (4)$$

where $N = N_d + N_c$. Equation (4) is the approximate completeness relation which is used in all GSM calculations.

Parallelization in the context of basis generation is meaningful only if one uses Hartree-Fock (HF) potentials, where one has to recalculate many times the one-body states of the basis, which can become lengthy as one can have tens of scattering states per partial wave contour. The use of HF potentials (or more generally of potentials tailored to the nucleus in consideration) has been seen to be necessary with the particular cases of ^8He [17] and the Li chain [13]. Indeed, the use of the basis generated by the core has been noticed to be insufficient, as the size of the nucleus changes significantly with the number of nucleons, so that convergence with the basis generated by the core potential becomes very slow compared to that of the HF basis. For the calculation of the basis, all nodes calculate all HF potentials independently, but calculate only part of the basis. Thus, MPI communication never occurs during the HF process, as it is only at the end of the calculation that HF potentials and wave functions are distributed to all nodes. However, OpenMP parallelization can be applied for the calculation of HF potentials, as it does not lead to communication overhead, the different points of HF potentials being calculated independently from each other.

3. Realistic interactions in GSM

The inclusion of nuclear realistic interactions (see [22, 23, 24, 25] for the ones most widely used) in GSM cannot be done directly, as in SM (see [26] where SM calculations using realistic interactions are effected for light nuclei), because the calculation of their matrix elements relies on the mathematical properties of the harmonic oscillator basis used in SM, absent from GSM. However, it is possible to expand the nuclear interaction only with harmonic oscillator states, even though the GSM matrix is represented with the Berggren basis. This is due to the finite-range character of the nuclear interaction, which is important only in the vicinity of the nucleus. The used nuclear interaction $\hat{V}$ writes using this method [14]:

$$\langle ab|\hat{V}|cd\rangle = \sum_{\alpha\beta\gamma\delta}^{N_{\max}} \langle\alpha\beta|\hat{V}|\gamma\delta\rangle \langle a|\alpha\rangle \langle b|\beta\rangle \langle c|\gamma\rangle \langle d|\delta\rangle, \quad (5)$$

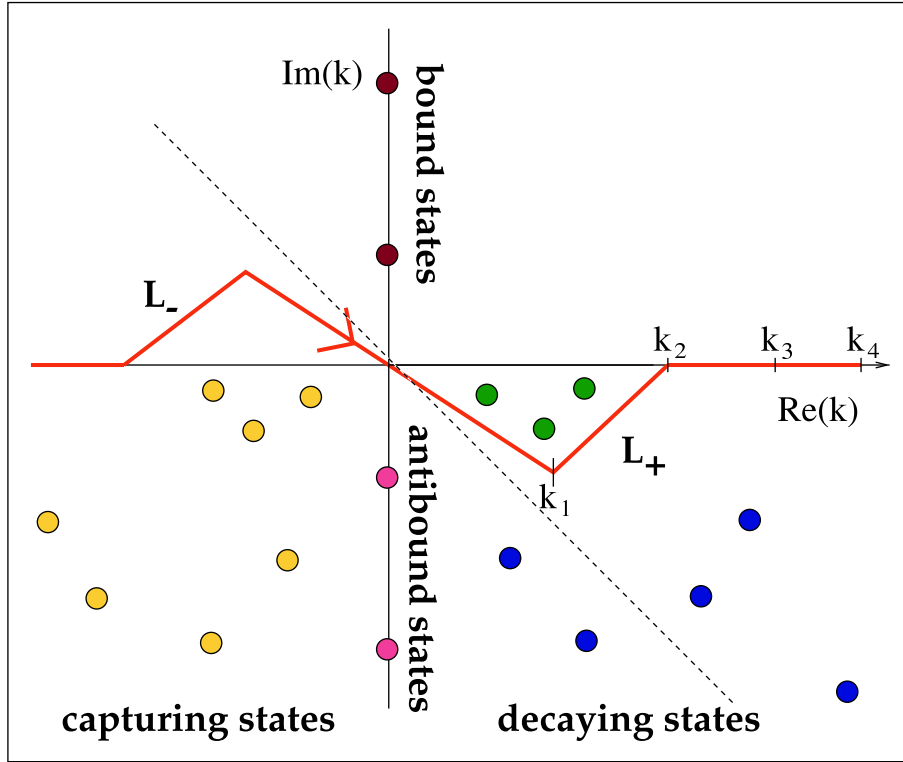


Figure 1. Complex plane of linear momenta k , where the positions of bound, resonant, antiresonant and antibound states are illustrated. L_+ is the contour of non-resonant states. The Berggren completeness relation includes bound states and the resonant states lying between the real axis and the L_+ contour. The L_+ contour must be chosen so that the poles of the discrete sum of (2) are enclosed between L_+ and the real k -axis.

where $N_{\max}$ is the number of harmonic oscillator states and Greek and Latin letters refer respectively to harmonic oscillator states and Berggren basis states. As $\hat{V}$ appears only in the right-hand side of (5) through matrix elements of harmonic oscillator states, the Moshinsky-Brody transformation can be used to calculate them. Berggren basis states can be found only in overlaps of the form $\langle a|\alpha\rangle$, necessitating no complex scaling as harmonic oscillator states always decrease like Gaussians for $r \rightarrow +\infty$ whereas Berggren basis states increase at most exponentially in modulus. Note that the one-body kinetic part of the Hamiltonian is directly expressed with the Berggren basis, hence without harmonic oscillator basis expansion, so that this scheme is not equivalent to a SM calculation.

This method has been applied to the ${}^6\text{He}$ and ${}^{18}\text{O}$ nuclei, modelled by two neutrons above a core, ${}^4\text{He}$ for ${}^6\text{He}$ and ${}^{16}\text{O}$ for ${}^{18}\text{O}$, using the N^3LO realistic interaction renormalized with the low-momentum interaction method [14]. The convergence of the energies of ground and excited states of the ${}^6\text{He}$ and ${}^{18}\text{O}$ nuclei, as well as that of the density of the halo state 0_1^+ of the ${}^6\text{He}$ nucleus, are illustrated respectively in Tabs.1,2 and figure 2. One notices therein that convergence is attained for $N_{\max} \sim 10$ in Tabs.1,2, and that even for resonant states. Moreover, the radial density of valence neutrons of the ground state of the ${}^6\text{He}$ nucleus corresponds to that of a halo state, as shown by linear and logarithmic scales (see figure 2, issued from [16]), which confirms the precision of the method. Hence, realistic interactions can be included in practice in the GSM formalism, which would be impossible without the decomposition described in (5).

Parallelization of the implementation of two-body matrix elements is trivial as they are all

calculated independently from each other. MPI is used for distribution of two-body matrix elements among nodes while OpenMP is used for the loop calculation of (5). Parallelization at this level is useful because, on the one hand, calculation of two-body matrix elements using firstly the Moshinsky-Brody transformation and secondly (5) is lengthy, and, on the other hand, the Berggren basis can contain tens of one-body basis states, so that the number of two-body matrix elements to calculate can be very large.

Table 1. Convergence of the energies of the 0_1^+ and 2_1^+ states of the ${}^6\text{He}$ nucleus as a function of the number of nodes of the harmonic oscillator states used in the expansion of the N^3LO interaction, renormalized with the low-momentum method. The momentum cut is effected at $\Lambda = 1.9 \text{ fm}^{-1}$ in the space of relative coordinates. The harmonic oscillator parameter is equal to $b = 2 \text{ fm}$. Energies are given in MeV.

n_{max}	$J^\pi = 0_1^+$		$J^\pi = 2_1^+$	
	Re[E]	Im[E]	Re[E]	Im[E]
4	-0.4760	0.0000	0.9504	-0.0467
6	-0.4714	0.0000	0.9546	-0.0461
8	-0.4719	0.0000	0.9597	-0.0453
10	-0.4721	0.0000	0.9602	-0.0452
12	-0.4721	0.0000	0.9600	-0.0452
14	-0.4721	0.0000	0.9601	-0.0452
16	-0.4721	0.0000	0.9601	-0.0453
18	-0.4721	0.0000	0.9601	-0.0453
20	-0.4721	0.0000	0.9601	-0.0453

Table 2. Same as in Tab.1, but for the $0_1^+, 0_2^+, 4_1^+$ and 4_2^+ states of the ${}^{18}\text{O}$ nucleus.

n_{max}	$J^\pi = 0_1^+$		$J^\pi = 0_2^+$		$J^\pi = 4_1^+$		$J^\pi = 4_2^+$	
	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]
4	-12.225	0.000	-8.438	0.000	-11.0641	0.0000	-1.4373	-0.8275
6	-12.226	0.000	-8.498	0.000	-11.0907	0.0000	-1.4292	-0.7600
8	-12.228	0.000	-8.499	0.000	-11.0922	0.0000	-1.4380	-0.7405
10	-12.229	0.000	-8.499	0.000	-11.0921	0.0000	-1.4400	-0.7390
12	-12.228	0.000	-8.499	0.000	-11.0923	0.0000	-1.4393	-0.7401
14	-12.228	0.000	-8.499	0.000	-11.0923	0.0000	-1.4394	-0.7401
16	-12.228	0.000	-8.499	0.000	-11.0923	0.0000	-1.4394	-0.7401
18	-12.228	0.000	-8.499	0.000	-11.0923	0.0000	-1.4394	-0.7401
20	-12.228	0.000	-8.499	0.000	-11.0923	0.0000	-1.4394	-0.7401

4. Diagonalization of giant GSM matrices with the density matrix renormalization group method

The presence of numerous scattering states in the Berggren basis within GSM generates very large valence space dimensions, which cannot be handled with Krylov methods, unless drastic truncations are imposed, as was the case for the first applications of GSM. In order to be able to determine eigenstates almost exactly in GSM, the DMRG method is being developed in the non-Hermitian case of GSM. The DMRG method originates from solid states physics [27] and allows to calculate eigenstates of matrices whose dimensions are beyond standard Krylov methods capabilities. It has been tested in nuclear physics in the frame of SM [28], and generalized to

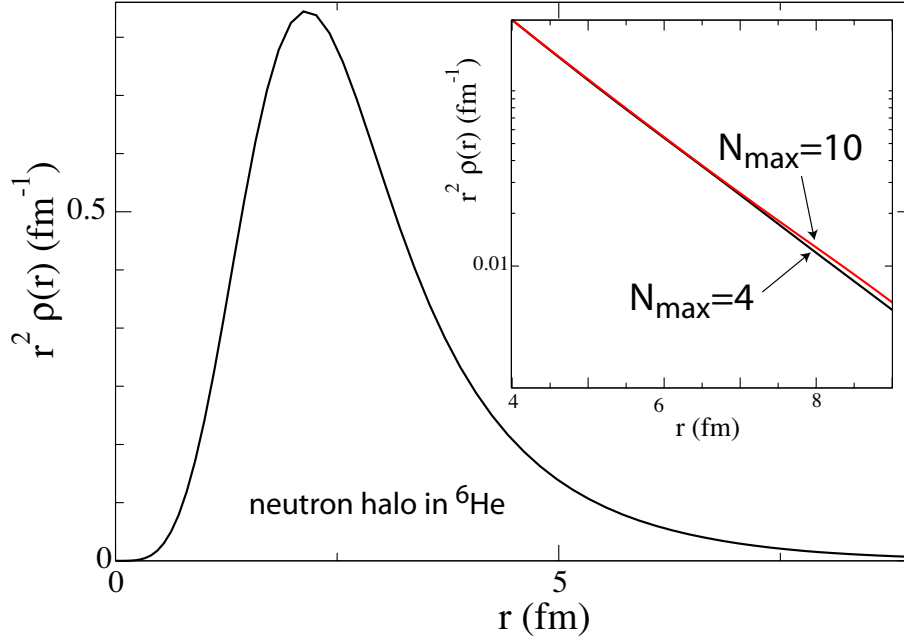


Figure 2. Radial density of valence particles of the ground state 0^+ of the ${}^6\text{He}$ nucleus for three different harmonic oscillator expansions of the nuclear interaction: $n_{\text{max}} = 4, 10$ and 16 . The asymptotic of the radial density is illustrated in the insert in logarithmic scale. Results for $n_{\text{max}} = 10$ and 16 are indistinguishable.

GSM firstly for a space of valence neutrons and then for GSM space containing both protons and neutrons afterwards [15].

The aim of this method is to build iteratively bases becoming more and more correlated, so that the GSM eigenstates can be expanded in a DMRG basis containing $N_d \sim 1000$ basis states [15]. For this, the GSM valence space is separated in two spaces A and B . The A space is constructed from the one-body resonant states of the Berggren basis, and from a few one-body non-resonant states of quantum numbers (ℓ, j) different from those of resonant states, necessary to generate all the possible couplings present in the Hamiltonian [15]. The B space is generated during the DMRG process, by adding one by one the remaining scattering states of the Berggren basis. Its elements are numbered by $i_B = 0, 1, \dots$. One then starts the "warm-up" phase [15]. For this, the configurations for all number of particles n_A and total angular momentum j_A , denoted as $|k_A\rangle$, are built in the A space, as well as all the associated suboperators of the Hamiltonian, whose list reads $a^\dagger$, $(a^\dagger \tilde{a})^K$, $((a^\dagger a^\dagger)^K \tilde{a})^L$, $(a^\dagger a^\dagger)^K (\tilde{a} \tilde{a})^K$, where $a^\dagger/\tilde{a}$ is a creation/annihilation operator and L, K angular momenta. Then, a new scattering shell (n, ℓ, j) is added, the configurations $|i_B\rangle$ for all possible number of particles n_B and total angular momentum j_B are constructed, which augments the size of the B space and generates a set of basis states $(|k_A(n_A, j_A)\rangle \otimes |i_B(n_B, j_B)\rangle)^J$, where $n_{A(B)}$ and $j_{A(B)}$ are respectively the numbers of particles and angular momenta of the $k_A(i_B)$ states and J is the total angular momentum of the calculated eigenstate. When the number of configurations i_B of the B space reaches N_{opt} , of the order of 10 to 100 typically, the Hamiltonian is diagonalized to provide an approximation of the calculated nuclear state:

$$|\Psi_J\rangle = \sum_{k_A, i_B} c_{i_B}^{k_A} \{|k_A\rangle \otimes |i_B\rangle\}^J, \quad (6)$$

where the Lanczos or Davidson method is used for diagonalization. $|\Psi_J\rangle$ of (6) has been

determined by the overlap method [11], which consists in diagonalizing firstly the GSM matrix without scattering basis states, so that a zeroth-order eigenstate can be determined with the Lanczos method, and secondly diagonalizing the full GSM matrix, whose sought bound or resonant eigenstate is the one which maximizes the overlap with the previously calculated zeroth-order eigenstate at pole approximation. The reduced density matrix $\rho_{i_B i'_B}^B$ is thus calculated from (6):

$$\rho_{i_B i'_B}^{j_B} = \sum_{k_A} c_{i_B}^{k_A} c_{i'_B}^{k_A}, \quad (7)$$

where the angular momentum j_B , which is the same for $|i_B\rangle$ and $|i'_B\rangle$, is fixed. The reduced density matrix is then diagonalized, and the resulting eigenvectors which possess the largest eigenvalues in modulus (at most N_{opt} of them) are kept in the model space, the other ones being rejected. This method is indeed motivated by the variational principle, which states that the wave function bearing the largest overlap with the exact nuclear state is the one built from the aforementioned eigenvectors [27]. The eigenvectors then generate the new B space, and the suboperators associated to the Hamiltonian are recalculated in this new space. When all the shells of the Berggren basis have been taken into account, the "warm-up" phase terminates and the "sweep" phases start [15]. They are similar to the "warm-up" phase, except that the states of the A space are now replaced by the $(|k_A(n_A, j_A)\rangle \otimes |i_B(n_B, j_B)\rangle)^J$ states, issued from the previous iteration. The scattering states (n, ℓ, j) of the Berggren basis are then reintroduced one by one, with the index associated to (n, ℓ, j) firstly decreasing ("sweep down") and afterwards increasing ("sweep up") [15]. Indeed, the truncation applied after each diagonalization of the reduced density matrix suppresses correlations, which must be recovered during sweeps. Convergence is obtained after a few "sweeps", of the order of five [15]. Every time a new scattering shell is added during a sweep, which translates into diagonalizations of new reduced density matrices and recalculations of Hamiltonian suboperators, by definition, a "step" occurs. The speed of convergence is measured via their number N_{step} .

The DMRG method has been tested with the calculation of the $3/2_1^-$ and $1/2_1^-$ eigenstates of ^7He and to the ground state of the ^7Li nucleus [15]. The convergence of the DMRG method is illustrated in Figs.3,4 for the ^7He and ^7Li nuclei. One can see that convergence is very rapid. The precision with respect to the number of discretized scattering states of the Berggren basis has also been studied (see figure 4). One can see that the energy and width of the ground state $3/2_1^-$ of the ^7He nucleus converge to a finite value, while the width of the ground state 0_1^+ of the ^6He nucleus goes to zero as the number of discretized scattering states of the basis increases, which is expected as the ground states of ^6He is bound. Even though it is bound, the ground state $3/2_1^-$ of the ^7Li nucleus has a non-zero width. The discretization of contours has indeed been chosen to be coarse for the ^7Li nucleus, so that GSM matrix dimensions are small enough so as to be able to calculate its ground state with the Davidson method and compare the exact result with that produced by the DMRG method. The imaginary part of the ground state of the ^7Li nucleus, which is bound, eventually disappears when the number of discretized scattering states augments [15].

The parallelization of the DMRG method has to be effected at two different levels, the first one at the level of the calculation of sub-operators (see above) and density/Hamiltonian matrix elements, and the second one at the level of the application of matrices on vectors. The latter is trivial to diagonalize. However, that of the sub-operators poses problem. Indeed, due to the numerous states of the Berggren basis, the matrix elements involving creation and annihilation operators become very large, contrary to standard shell model, where the proton and neutron parts of the Hamiltonian can be fully stored and hence efficiently handled, the proton-neutron part of the Hamiltonian taking virtually all the time of calculation [1]. For neutron-rich nuclei, for which the Berggren basis consists mainly of discretized neutron contours, the neutron part is

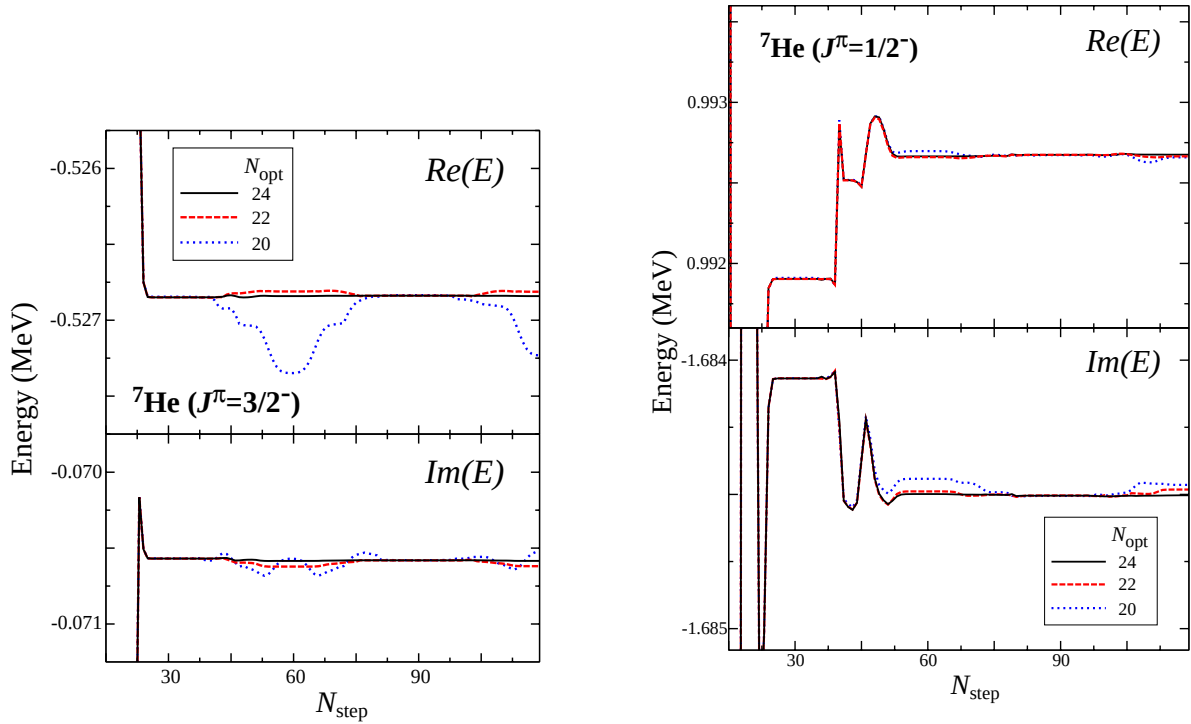


Figure 3. Convergence of the real (upper part) and imaginary (lower part) parts of the energy of the ground state $3/2^-$ (left) and excited state $1/2^-$ (right) of the ${}^7\text{He}$ nucleus as a function of N_{step} for several values for N_{opt} (see text for their definition).

the most expensive to treat, proton and proton-neutron parts being secondary, if not negligible. The parallelization of the calculation of sub-operators is by itself trivial to consider as they are independent from each other. However, due to their number, they must be stored on hard disk, and the parallelization of input/output has not yet been done, due to the complex distribution of used sub-operators matrix elements in the generation of the Hamiltonian matrix. Hence, the saving and loading of sub-operators matrix elements is for the moment the bottleneck of the DMRG method as it is coded now, as calculations demanding more than six valence particles are precluded. The parallelization of the input/output process is currently investigated.

5. Conclusion

Exotic nuclei, begin OQSs, are radically different from stable nuclei, of CQS nature. Hence, they must be studied with models incorporating their uncommon features, for example the presence of a halo or resonant character at ground state level. For this, the Gamow Shell Model has been developed, which makes use of the Berggren basis, with which the direct inclusion of bound, resonant and scattering states allows to describe the long-range character of the many-body wave functions of nuclei far from the valley of stability. However, the mathematical properties of the standard harmonic oscillator basis being absent in the Berggren basis, a new mathematical method had to be developed in order to calculate efficiently the matrix elements of the nuclear interaction in the Berggren basis. The most difficult part to handle in this model is the diagonalization of matrices much larger than in SM, as the Lanczos and Davidson are insufficient to treat such large dimensions. For this, the DMRG has been proved to be able to

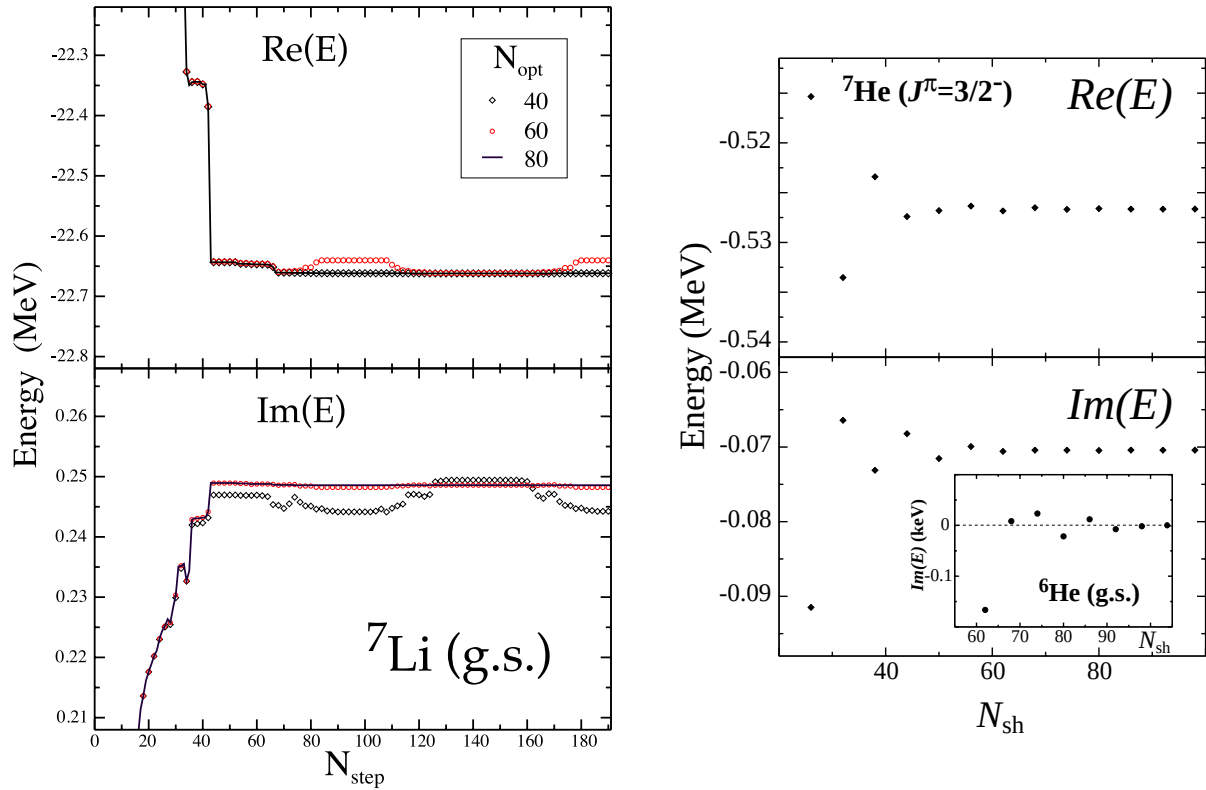


Figure 4. On the left, same as figure 3, but for the ground state $3/2^-$ of the ${}^7\text{Li}$ nucleus. On the right, the convergence of the energy (upper part) and width (lower part) of the ground state $3/2^-$ of the ${}^7\text{He}$ nucleus as a function of the number of discretized scattering states of the Berggren basis is depicted. The width of the ground state 0_1^+ of the ${}^6\text{He}$ nucleus as a function of the number of discretized scattering states of the Berggren basis is shown in the insert of the lower part.

solve this problem. While parallelization of introduced methods can usually be effected without difficulty, the necessary disk input/output of large tables in the DMRG is, on the contrary, problematic for that matter. This problem will have to be solved in order to be able to consider more valence particles with this powerful method.

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