Ab Initio Description of Light Nuclei in the Berggren Basis

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Abstract

In this work we report on the first application of the No-Core Gamow Shell Model to study *ab initio* bound and unbound states in light nuclei. This model is formulated in the complex energy plane by using a complete Berggren ensemble which treats bound, resonant, and scattering states on equal footing. The resolution of the many-body Schrödinger equation is performed with the technique of the Density Matrix Renormalization Group.

Keywords: *Ab initio method; coupling with the continuum; Density Matrix Renormalization Group*

1 Introduction

In the last decade our knowledge of nuclei far from the valley of stability has radically improved. This improvement has been a by-product of advances in both experiment and theory. New experimental facilities that have already been built (RIBF at RIKEN) or are being constructed (SPIRAL2 at GANIL, FAIR, FRIB at MSU) will give us a better insight of areas in the nuclear chart that have never been explored, pushing even further our knowledge at the limits of nuclear existence. At the same time, the increase in computing power has made it possible to calculate properties of nuclei in an *ab initio* fashion, using realistic interactions which reproduce nucleon-nucleon scattering data. For few-body systems ($A \leq 4$) methods such as Faddeev [1] and Faddeev–Yakubovsky (FY) [2] provide an exact solution to the many-body problem. Methods such as the Green's Function Monte Carlo (GFMC) [3], the Hyperspherical Harmonics [4], the No-Core Shell Model (NCSM) [5], the Coupled-Cluster (CC) approach [6] and more recently, the In-Medium Similarity Renormalization Group method [7] and Dyson Self-Consistent Green's Function method [8] have been applied successfully for the *ab initio* description of light and medium mass nuclei.

Nuclei with large isospin which can be found in these remote regions, have attracted a great deal of interest. They belong to the category of Open Quantum Systems, inter-connected via the decay and reaction channels. These are very fragile objects with small separation energies and very large spatial dimensions. The proximity of the continuum affects their bulk properties (matter and charge distributions) and their spectra. Phenomena such as the anomalous behavior of elastic cross-sections and the associated overlap integral near threshold states in multi-channel coupling (Wigner-cusps) [9] and the appearance of cluster correlations in the vicinity of the respective cluster emission threshold [10], to mention a few, are all unique manifestations of the continuum coupling.

From the theoretical perspective, existing many-body methods have had to be generalized in order to construct approaches where both structure and reactions are unified to describe these exotic systems. Examples of these attempts are the Shell Model

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Embedded in the Continuum (SMEC) [11] and the Gamow Shell Model (GSM) [12,13] in which nuclei are described as systems with a core above which valence nucleons interact. The GSM, which is the most recent of these two approaches, is a generalization of the Harmonic Oscillator (HO) shell model in the complex energy plane using the Berggren ensemble [14]. Recent *ab initio* approaches such as the NCSM coupled with the Resonating Group Method [15], the CC approach generalized in the complex-energy plane using the Berggren basis [16] and the GFMC [17], have allowed an *ab initio* description of bound and unbound states of nuclei.

In this work we introduce the No-Core Gamow Shell Model (NCGSM) [18] as an alternative for *ab initio* calculations of weakly-bound and unbound states of light nuclei using realistic interactions. We will show the basic ingredients of the NCGSM and describe the many-body method namely, the Density Matrix Renormalization Group (DMRG) technique, used to solve the many-body problem. We will then present selected results obtained in this approach.

2 Formalism

The intrinsic Hamiltonian H for a nucleus with A nucleons is given by

$$H = \frac{1}{A}\sum_{i<j}^{A}\frac{(\vec{p}_i - \vec{p}_j)^2}{2m} + \sum_{i<j}^{A} V_{ij}^{NN}, \tag{1}$$

where m is the nucleon mass, $\vec{p}_i$ is the momentum of the nucleon i and V^{NN} is a two-body nuclear potential. In the NCGSM [18], the weakly-bound/unbound eigenstates of H are obtained by using an expansion in the Berggren basis which allows to treats bound, resonant and scattering states on equal footing. Let us consider a finite-depth single-particle (s.p.) potential. Its eigenstates fulfill the Berggren completeness relation which can be written as

$$\sum_{n=b,d} |u_n\rangle\langle\widetilde{u_n}| + \int_{L_+} |u_k\rangle\langle\widetilde{u_k}|\, dk = 1, \tag{2}$$

where b are bound states, d are decaying resonant states and the integral along a contour L_+ represents the contribution from the non-resonant scattering continuum, see Fig. 1. By discretizing the integral in (2), a discrete set of s.p. states can be obtained from which one constructs the many-body basis in which the Hamiltonian H is diagonalized. Due to the inclusion of resonant states and complex-continuum states, the representation of H in the (many-body) Berggren basis is complex-symmetric. The dimension of the Hamiltonian matrix grows rapidly with the number of discretized continuum states and nucleons and as a consequence, advanced numerical methods that can handle large non-Hermitian matrices must be used. In the context of the GSM, it has been shown that the DMRG method is an efficient way to compute the low-lying spectrum of the Hamiltonian at a low computational cost [13, 19]. In the following, we describe the main features of DMRG applied to the NCGSM.

The DMRG method was first introduced to overcome the limitations of the Wilson-type renormalization group to describe strongly correlated systems with short-range interactions [20]. More recently, the DMRG has been reformulated and applied to finite Fermi systems [21], nuclear shell model [22–24], and open systems [19]. While most of the DMRG studies have been focused on properties in strongly correlated closed quantum systems characterized by Hermitian density matrices, systems involving non-Hermitian and non-symmetric density matrices can also be treated [19, 25].

Let us consider the application of the J-scheme DMRG in the context of the NCGSM. The objective is to calculate an eigenstate $|J^\pi\rangle$ of the Hamiltonian $\hat{H}$ with angular momentum J and parity π. As $|J^\pi\rangle$ is a many-body pole of the scattering

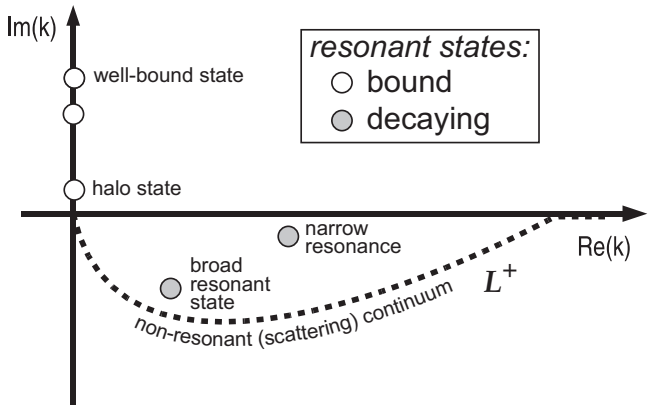

Figure 1: Illustration of the Berggren completeness relation (2) in the complex k-plane. The bound states are located on the positive imaginary axis. The weakly bound halo states lie close to the origin. The positive-energy resonant states are located in the fourth quadrant. Those with a small imaginary part can be interpreted as resonances. The complex-k contour L^+ represents the non-resonant scattering continuum.

matrix of $\hat{H}$, the contribution from non-resonant scattering shells along the continuum contour L^+ to the many-body wave function is usually smaller than the contribution from the resonant orbits [12]. Based on this observation, the following separation is usually performed [19]: the many-body states constructed from the single-particle poles form a subspace A (the so-called 'reference subspace'), and the remaining states containing contributions from non-resonant shells form a complement subspace B (see Fig. 2).

One begins by constructing states $|k\rangle_A$ forming the reference subspace A. All possible matrix elements of suboperators of the GSM Hamiltonian $\hat{H}$ acting in A, expressed in the second quantization form, are then calculated and stored and the Hamiltonian is diagonalized in the reference space to provide the zeroth-order approximation $|\Psi_J\rangle^{(0)}$ to $|J^\pi\rangle$. The scattering shells (lj), belonging to the discretized contour L^+, are then gradually added to the reference subspace to create the subspace B. This first stage of the NCGSM+DMRG procedure is referred to as the 'warm-up phase'. For each new added shell, all possible many-body states denoted as $|i\rangle_B$ are constructed and matrix elements of suboperators of the Hamiltonian H acting on $|i\rangle_B$ are computed. By coupling states in A with the states $|i_B\rangle$, one constructs the set of states of a given J^π. This ensemble serves as a basis in which the NCGSM

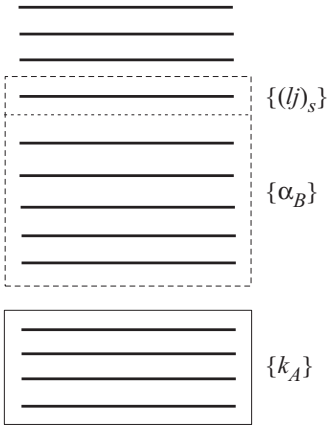

Figure 2: Schematic illustration of the NCGSM+DMRG procedure during the s^{th} step of the warm-up phase. States $\{k_A\}$ from A, previously optimized states α_B, and states $\{(lj)_s\}$ constructed by occupying the s^{th} shell with n particles are coupled to generate the new set of states $\{k_A \otimes i_B\}^J = \{k_A \otimes \{\alpha_B \otimes (lj)^n_s\}\}^J$.

Hamiltonian is diagonalized. The target state $|\Psi_J\rangle$ is selected among the eigenstates of $\hat{H}$ as the one having the largest overlap with the reference vector $|\Psi_J\rangle^{(0)}$. Then, the desired truncation is performed in B by introducing the reduced density matrix, constructed by summing over the reference subspace A [26]. In standard DMRG applications for Hermitian problems, where the eigenvalues of the density matrix are real non-negative, only the eigenvectors corresponding to the largest eigenvalues are kept during the DMRG process. Within the metric defining the Berggren ensemble, the NCGSM density matrix is complex-symmetric and its eigenvalues are, in general, complex. As a consequence, the truncation is done by keeping the eigenstates α_B (the 'optimized' states) with the largest nonzero moduli of eigenvalue [19]. The trace of the density matrix being equal to one, the truncation is done by keeping eigenstates of the density matrix with the corresponding eigenvalue w_α such that the condition

$$\left| 1 - Re\left(\sum_{\alpha=1}^{N_\rho} w_\alpha \right) \right| < \epsilon \tag{3}$$

is satisfied. The quantity ϵ in (3) can be viewed as the truncation error of the reduced density matrix. The smaller ϵ, the larger number of eigenvectors must be kept. In particular, for ϵ=0, all eigenvectors with non-zero eigenvalues are retained.

The warm-up phase is followed by the so-called sweeping phase, in which, starting from the last scattering shell $(lj)_{\text{last}}$, the procedure continues in the reverse direction (the 'sweep-down' phase) until the first scattering shell is reached. The procedure is then reversed and a sweep in the upward direction (the 'sweep-up' phase) begins. The sweeping sequences continue until convergence for target eigenvalue is achieved.

3 Selected results

We now show few results obtained with the NCGSM+DMRG approach and we start here with the ground state in ^{4}He. Obviously this system is well-bound and can be described using an expansion in a HO basis without including continuum states. Nevertheless, using an expansion in the Berggren basis in that case allows to test our approach by comparing with exact results obtained in the Faddeev–Yakubovsky approach [1]. The two-body interaction V^{NN} in (1) is chosen as the Argonne v_{18} interaction renormalized with the V_{low-k} method [27] with a sharp momentum cutoff $\Lambda = 1.9$ fm^{-1}. Using this renormalization scheme allows a decoupling between high-momentum and low-momentum degrees of freedom and as a consequence, improves the convergence of nuclear structure calculations [27]. We include $s_{1/2}$, $p_{3/2}$, $p_{1/2}$, $d_{3/2}$, $d_{5/2}$, $f_{7/2}$, $f_{5/2}$, $g_{9/2}$, $g_{7/2}$ shells for protons and neutrons. For the partial waves with angular momentum $l \leq 1$, the s.p. basis is generated by performing Gamow–Hartree–Fock (GHF) [12] calculations. In this case, the GHF potential has a neutron and proton bound state in the $s_{1/2}$ channel at respectively -26.290 MeV and -24.453 MeV. The rest of s and p shells are taken along the contour on the real k-axis which extends up to 4 fm^{-1} and is discretized with 18 points. For shells with $l \geq 2$, we take the HO basis functions given by a HO potential with a radius $b = 1.5$ fm and we include 5 d, 3 f and 3 g s.p. states for both protons and neutrons. Results for the g.s. energy in ^{4}He are shown in Fig. 3 as a function of the iteration of the NCSM+DMRG method for a truncation $\epsilon = 10^{-6}$. One can see that, as the middle of the third sweep is reached, the energy has converged and the corresponding value is

$$E_{\text{NCGSM}} = -29.15 \text{ MeV},$$

whereas the exact result in the FY approach [1] is

$$E_{\text{FY}} = -29.19 \text{ MeV}.$$

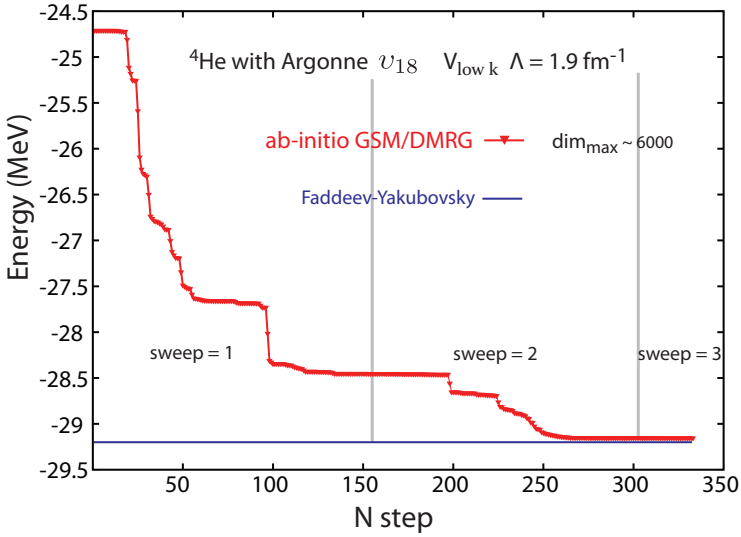

Figure 3: Energy of the ground state in ^{4}He as a function of the number of step ($N_{\rm step}$). Comparison of the NCGSM with the FY result with the V_{low-k} Argonne υ_{18} interaction.

The largest Hamiltonian matrix one has to deal with in the NCSM+DMRG has a dimension $D_{\rm max} \sim 6000$ whereas a direct resolution of the NCSM Hamiltonian matrix, that is for $\epsilon = 0$, would require to diagonalize a matrix of dimension 6,230,512 in J-scheme. The difference between our theoretical result and the experimental binding energy $E^{exp} = -28.30$ MeV, is due to higher-order terms in the nuclear interactions, such as three-nucleon forces, which are not included in the Hamiltonian (1).

We now show results for the ^{5}He nucleus which is a challenge for any many-body theory because of its unbound character. In particular, both the ground and first excited states are many-body resonances. Because of these characteristics, the complex energy formulation of the NCGSM using the Berggren ensemble is a perfect tool for its description. Indeed, in our formalism the resonance parameters (g.s. energy with respect to ^{4}He and the width) will be identified as the eigenvalues of the complex-symmetric Hamiltonian matrix. The position of the resonance will then be the real part of the energy, while the imaginary part is related to the width by the formula: $\Gamma = -2\,\Im{\rm m}(E)$. We use here the N^{3}LO interaction renormalized by V_{low-k} with a cutoff $\Lambda = 1.9$ fm^{-1}. For $l \leq 1$, the s.p. basis for protons and neutrons are generated by the GHF potential. In the $l = 0$ partial wave there are two bound states at $E = -23.290$ MeV and $E = -23.999$ MeV for respectively neutron and proton. The GHF potential has a $p_{3/2}$ s.p. resonance with a real part of energy 1.193 MeV and a width 1267 keV. In order to fulfill Berggren completeness, the $p_{3/2}$ contour is taken in the fourth-quadrant of the complex k-plane (see Fig. 1) whereas the $s_{1/2}$ and $p_{1/2}$ contours are chosen along the real-k axis. For states with $l \geq 1$, the s.p. states are given by HO basis functions as previously for ^{4}He. In Figs. 4, 5 we show the NCGSM+DMRG convergence pattern, for a truncation $\epsilon = 10^{-6}$, of the real and imaginary parts of the g.s. energy in ^{5}He. In the middle of the third sweep, the energy has converged to

$$\Re{\rm e}(E_{\rm NCGSM}) = -26.31 \text{ MeV}, \qquad \Im{\rm m}(E_{\rm NCGSM}) = -0.2 \text{ MeV}.$$

The real part lies at about 1 MeV above the experimental total binding energy [28] and as previously, the difference with the experimental binding energy is due to omitted higher-order terms in the nuclear interactions. For this truncation, the largest Hamiltonian matrix that needs to be diagonalized during the DMRG iterations has a

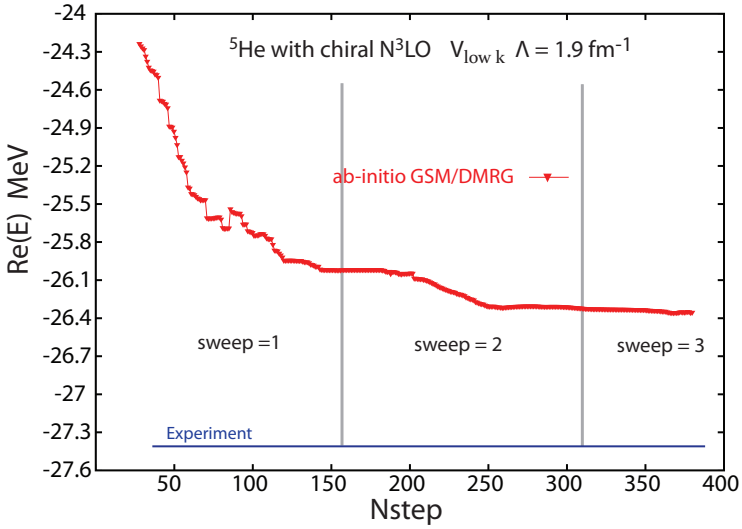

Figure 4: Real part of the energy of the ground state in ^{5}He as a function of the number of step ($N_{\rm step}$) using the chiral N^{3}LO interaction renormalized by by V_{low-k} with $\Lambda = 1.9$ fm^{-1}.

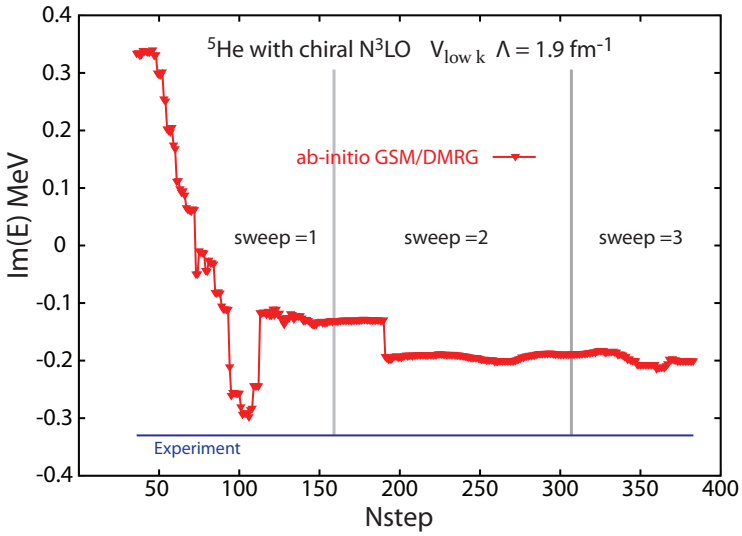

Figure 5: Imaginary part of the energy of the ground state in ^{5}He as a function of the number of step ($N_{\rm step}$) using the chiral N^{3}LO interaction renormalized by by V_{low-k} with $\Lambda = 1.9$ fm^{-1}.

dimension $D_{\rm max}$ $\sim 10^5$, whereas in the case of the full diagonalization i. e. for $\epsilon = 10^{-6}$, the Hamiltonian matrix has a dimension $\sim 3 \times 10^9$.

4 Summary

We have presented an *ab initio* approach to describe bound/unbound light nuclei using the framework of the No-Core Gamow Shell Model (NCGSM). By working in the Berggren ensemble, the NCGSM allows bound, resonant and scattering states to be treated on equal footing. The numerical solutions of the many-body Schrödinger equation are obtained by applying the Density Matrix Renormalization Group (DMRG)

method. We have shown results for the ground state in ^{4}He (bound nucleus) and the many-body ground state resonance in ^{5}He. This work serves as a proof of principle of the application of the Berggren's basis in a NCSM framework. In the future, we plan to apply the NCGSM+DMRG to study the structure of weakly bound/unbound light systems as for instance the very exotic systems in the hydrogen isotopic chain.

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