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State-dependent interactions for the Gamow shell model

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Abstract

A momentum space representation of the Berggren completeness is used in Gamow shell model calculations of the $^{5-7}$He isotopes. A major problem in the newly developed Gamow shell model is the extreme growth of the number of many-body configurations as the number of valence particles increases. This problem is addressed using the Lee–Suzuki similarity transformation method in the construction of an effective two-body interaction. At the convergence the dimensionality is found to be drastically reduced as compared to the full problem. This offers a promising approach to the study of weakly bound nuclei.

Tanihata's discovery in 1985 [1] of spatially extended nuclei (^{6,8}He; ^{11}Li; ^{11}Be) at the neutron dripline has over the last two decades triggered interest in the study of weakly bound and resonance phenomena in few-body systems. A proper shell model (SM) description of loosely bound nuclei should take into account the coupling of the discrete bound states with the continuum of positive scattering states. This coupling has been neglected in most modern *ab initio* approaches. The coupling of the external continuum of positive energy states, with the internal nuclear states, has however for a long time been basic ingredients in nuclear reaction theory, Feshbach being the first to formulate a unified description of direct and compound nuclear reactions within the projection operator method [2, 3]. He showed that the coupling of the internal with the external environments could give rise to compound nuclear states, such as multi-channel resonances. As he was the first to formulate a general theory of such states, they have become known as Feshbach resonances. Also in atomic physics, Feshbach resonances are of great importance. In fact, in the early 1960s, at the time of Feshbach's work, Fano [4] discussed how mixing of a configuration belonging to a discrete spectrum with configurations belonging to a continuous spectrum gives rise to the phenomena of *autoionization*, which is considered a multi-channel resonance or in other words a Feshbach resonance.

Aiming at realistic structure calculations of weakly bound nuclei, a unification of standard structure and reaction theory seems to be in place. If the SM is to be a reliable theory of such

loosely bound or unbound systems, a reformulation using a single-particle representation where the continuum is properly taken into account has to be searched for. In the late 1960s Berggren proved that for a finite range potential, a finite set of bound and resonant states together with a set of non-resonant continuum states form a complete set [5] of bi-orthogonal functions. In the Berggren ensemble bound, anti-bound, resonant and the non-resonant continuum states are treated on equal footing, so the Berggren basis seems to be a viable starting point for SM calculations of weakly bound and/or unbound nuclei. The newly developed Gamow shell model (GSM) is devoted to such an approach (see, for example, [6–14]). Starting with the discretized single-particle Berggren representation [5, 15–19], a complete anti-symmetrized many-body Berggren basis may be constructed. This is in full analogy with the standard SM which uses a harmonic oscillator basis. Expanding the many-body wavefunctions in this complete set of Berggren Slater determinants, allows for an interpretation of exotic multi-particle structures in terms of single-particle resonances. In this respect, the GSM may provide an answer to the question of how exotic structures near the dripline, such as multi-particle resonances embedded in the continuum, are formed.

The GSM is in its early stages, and so there exist a vast area of application and major theoretical and computational challenges to be dealt with. One of the first challenges and problems encountered in the GSM, is the *identification problem*, first addressed in [9, 10]. The physical multi-particle resonances will in many cases be embedded in a dense distribution of continuum states, depending on the contour on which the continuum states are defined. References [9, 10] relate this *identification problem* to the problem of choosing a contour in the complex k-plane which in the case of several valence particles selects the physical interesting states from the dense continuum background. They found that in the case of two valence particles, choosing a *square-well* contour makes an identification of physical states, based on inspection of the zeroth order energy surface possible. This solution is only applicable in the two-particle case, since already in the three-particle case the pole configurations get mixed in with the continuum configurations. In [7, 11, 12] the problem of identifying multi-particle resonances was approached from a different angle. The proposed algorithm is a two-step procedure. First a diagonalization within the pole space, where all particles are in resonant single-particle orbitals, is performed. Secondly a diagonalization within the complete configuration space is performed. Under assumption of weak coupling of the pole configurations with the configurations where at least one particle moves in a continuum orbital, the physical states may be picked out unambiguously from the states obtained after a full diagonalization, using the criterion of largest overlap with the pole space. The weak coupling limit may not always be a valid assumption, as pointed out in [14] for the case of ^{11}Li, the two-particle resonances may have a larger continuum component as compared to the pole component, depending on the strength of the residual nucleon–nucleon interaction. Thus, one may conclude that the *identification problem* has not been solved generally, and developing an algorithm which picks out physical states unambiguously from the dense continuum background is still an open problem.

Another challenge for the GSM is the *dimensionality problem*, which is the main topic of this paper. As the number of active particles moving in a valence space increases, the number of Slater determinants in the many-body Berggren basis increases dramatically. This explosion of many-body configurations is in the GSM approach even more severe than in the standard SM where only bound states appear. In the GSM one has for each partial wave a finite number of non-resonant continuum states which is absent in the standard SM. In handling *dimensionality problem*, one takes advantage of effective operator and perturbation method techniques typically used and developed for large scale SM calculations using harmonic oscillator bases.

In this work we consider as a test the light drip-line nuclei ^{5,6,7}He, and the formation of resonances in these nuclei. These nuclei have also been studied with a number of other methods (see, for example, [20], and references therein). We construct a single-particle basis using the contour deformation method in momentum space, discussed in detail in [19], which is used in constructing a complete set of two- and three-particle Slater determinants. Our solution to the *dimensionality problem* is a compromise between the inspection method used in [9, 10] and the overlap method used in [7, 11, 12]. We show that choosing a rotated plus translated contour in the complex plane, a large portion of the zeroth-order many-particle energy surface is free from complex continuum states. So in this respect an identification based on inspection of the zeroth-order energy spectrum is possible, by studying how the two- and three-particle resonances develop as the nucleon–nucleon interaction is gradually turned on. In going beyond two valence particles, we divide the complete many-body space in two sub-spaces, a model and a complement space. In the case of the three-particle resonances in ^{7}He, we construct an effective interaction at the two-body level in the model space. The model space is chosen optimally, and the effective interaction takes into account the most important many-body correlations, giving a much faster convergence with increasing model space as compared with the 'bare' interaction.

The outline of the paper is the following. In section 1, we present the results of the energy spectra of the $^{5-7}$He isotopes using the bare interaction and performing a full diagonalization. In section 2, the Lee–Suzuki similarity transformation method is presented, and generalized to complex interactions. A convergence study of the $3/2^-$ ground state of ^{7}He using the bare and the effective interaction is given. Section 3 gives the conclusions of the present study and future perspectives and challenges for GSM calculations.

1. Gamow shell-model calculations of the $^{5-7}$He isotopes

1.1. ^{5}He single-particle basis using the contour deformation method

In [19] we studied the contour deformation method applied to the momentum space Schrödinger equation. It was discussed and shown how the specific choices of contours based on the analytic structure of the potential may allow for a unified description of bound, anti-bound (virtual) and resonant states. Here, and in [21], CDM is the basic starting point for obtaining a single-particle Berggren basis for use in GSM calculations.

The analytically continued Schrödinger equation on a general inversion symmetric contour takes the form

$$\frac{\hbar^2}{2\mu}k^2\psi_{nl}(k) + \frac{2}{\pi}\int_{C^+} \mathrm{d}q\, q^2 V_l(k,q)\psi_{nl}(q) = E_{nl}\psi_{nl}(k), \tag{1.1}$$

where both k and q are defined on an inversion symmetric contour C^+ in the lower half complex k-plane, resulting in a closed integral equation. The eigenfunctions constitute a complete bi-orthogonal set, normalized according to the Berggren metric [5, 15–18], namely

$$\mathbf{1} = \sum_{n\in\mathbf{C}} |\psi_{nl}\rangle\langle\psi^*_{nl}| + \int_{C^+} \mathrm{d}k\, k^2 |\psi_l(k)\rangle\langle\psi^*_l(k)|. \tag{1.2}$$

This work uses a single-particle Berggren basis defined on a rotated plus translated contour, C^+_{R+T}, in the complex k-plane, studied in detail in [19]. The contour C^+_{R+T} is part of the inversion symmetric contour $C_{R+T} = C^+_{R+T} + C^-_{R+T}$ displayed in figure 1. The complete set of single-particle orbits defined by this contour will then include anti-bound, bound and resonant states, and serves as starting point for GSM calculations.

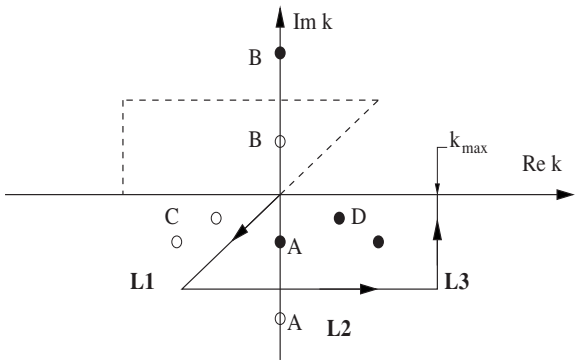

Figure 1. Contour $C^{+}_{R+T} = L_1 + L_2 + L_3$ is given by the solid line, while the contour C^{-}_{R+T} is given by the dashed line. The contour $C_{R+T} = C^{+}_{R+T} + C^{-}_{R+T}$ is inversion symmetric. The single-particle spectrum which is exposed by this contour is marked by filled circles • and the excluded spectrum by open circles ○. The full spectrum includes bound states (B), anti-bound (A), decay (D) and capture (C) resonant states.

Turning now to the application of CDM to the unbound nucleus ^{5}He. This nucleus may be modelled by an inert ^{4}He core with a neutron moving mainly in the resonant spin–orbit partners $p_{3/2}$ and $p_{1/2}$. The $J^\pi = 3/2^-_1$ resonance, to be associated with the single-particle orbit $p_{3/2}$, is experimentally known to have a width of $\Gamma \approx 0.60$ MeV while the $J^\pi = 1/2^-_1$ resonance, associated with the single-particle orbit $p_{1/2}$, has a large width $\Gamma \approx 4$ MeV. For more information on these systems, see for example the recent review by Jonson [20]. The core-neutron interaction in ^{5}He may be phenomenologically modelled by the SBB (Sack, Biedenharn and Breit) potential [22]. The SBB potential is of Gaussian type with a spin–orbit term, fitted to reproduce the neutron—^{4}He scattering phase shifts.

In the complex k-plane the Gaussian potential diverges exponentially for $|\mathrm{Im}[k]| > |\mathrm{Re}[k]|$. If we apply the complex scaling technique, which consists of solving the momentum space Schrödinger equation on a purely rotated contour, we get the restriction $\theta < \pi/4$ on the rotation angle (clockwise). Even for smaller angles we may get a poor convergence, since the Gaussian potential oscillates strongly along the rotated contours. On the other hand, choosing a contour of the type C^{+}_{R+T} solves this problem, allowing for a continuation in the third quadrant of the complex k-plane. Furthermore, it yields a faster and smoother decay of the Gaussian potential along the chosen contour.

Since ^{5}He has only resonances in its spectrum, namely, no anti-bound states, there is no need for an analytic continuation in the third quadrant of the complex k-plane, as done in [19] for the free nucleon–nucleon interaction. We choose a contour of the type C^{+}_{R+T} rotated with $\theta = \pi/4$ and translated with $|\mathrm{Im}[k]| = 0.4 \sin(\pi/4) \approx 0.28$ fm^{-1} in the fourth quadrant of the complex k-plane.

Table 1 gives the convergence of the $p_{3/2}$ and the $p_{1/2}$ single-particle resonances as function of integration points along the contour C_{R+T}. We observe that with 12 points along the rotated path and 12 points along the translated line, one has a reasonable convergence of the $3/2^-$ and $1/2^-$ resonance energies. Note also that the calculated width of the $1/2^-$ resonance is somewhat larger (≈ 6 MeV) than the experimental value (≈ 4 MeV), see [20].

1.2. Two- and three-particle resonances in $^{6-7}$He

In the following we limit the valence space to the $p_{3/2}$ shell only. The reason we do not include the $p_{1/2}$ single-particle orbits is that we aim at a diagonalization in the full space, taking into

Table 1. Convergence of $p_{3/2}$ and $p_{1/2}$ resonance energies in ^{5}He as a function of the number of integration points N_R along the rotated C_R and N_T along the translated part C_T of the contour. Energies in MeV.

		$J^\pi = 3/2^-$		$J^\pi = 1/2^-$	
N_R	N_T	Re(E)	Im(E)	Re(E)	Im(E)
10	10	0.752 321	−0.329 830	2.148 476	−2.912 522
12	12	0.752 495	−0.327 963	2.152 992	−2.913 609
20	20	0.752 476	−0.328 033	2.154 139	−2.912 148
30	30	0.752 476	−0.328 033	2.154 147	−2.912 162
40	40	0.752 476	−0.328 033	2.154 147	−2.912 162

account all complex continuum couplings. First we present results for the resonant spectra of ^{6}He, employing again a SM picture with ^{6}He modelled by an inert ^{4}He core and two valence neutrons moving in the $p_{3/2}$ orbits. The recoil of the core has been ignored in all calculations. The model space consists then of all momenta k defined by the set of mesh points along the contour. Using the single-particle wavefunctions for ^{5}He of subsection 1.1, an N-body anti-symmetric wavefunction can be constructed namely,

$$\Psi_\alpha^{JM}(1,\ldots,N) = \sum_i C_i^{JM}\Phi_i^{JM}(1,\ldots,N), \tag{1.3}$$

where the indices i represent the various single-particle orbits. Here $\Phi_i^J(1,\ldots,N)$ is a normalized N-body anti-symmetric wavefunction. In our case we have $N = 2$ for ^{6}He and $N = 3$ for ^{7}He, respectively. The sum over single-particle orbits is limited by $a \leqslant b \leqslant c \ldots$ since we deal with identical particles only.

As an effective two-neutron interaction V_{ij} we use a phenomenological interaction of Gaussian type, separable in $\mathbf{r}_i, \mathbf{r}_j$ and with interaction strength V_0, given by

$$V_{ij}(\mathbf{r}_i, \mathbf{r}_j) = V_0 \exp\left(-\frac{\left(r_i^2 + r_j^2\right)}{a^2}\right) \sum_\lambda (Y_\lambda(i) \cdot Y_\lambda(j)). \tag{1.4}$$

The interaction strength is fitted to reproduce the 0^+ binding energy in ^{6}He. We have observed that the position of the 2^+ resonance in ^{6}He depends on the range a of the Gaussian interaction, even though we fit the strength so that the 0^+ ground state does not change with a. Unfortunately it turns out that for larger values of a the energy fit is better, but the convergence as a function of mesh points is poorer. This demonstrates that the two-particle resonant spectrum depends strongly on the radial shape of the interaction and suggests that we should rather deal with an effective interaction derived from realistic models for the nucleon–nucleon interaction. In our calculations we have chosen a value of a which is a compromise between a small number of mesh points along the contour and a reasonable good fit of the resonant energy spectra. The parameters used in our calculations are $V_0 = -5.315$ MeV and $a = 4.8$ fm, for the model space involving only the ($p_{3/2}$) orbitals.

The stability of the 0^+ and 2^+ results as function of the number of mesh points is demonstrated in table 2. We note that with $N_R = 12$ integration points along the rotated path C_R and $N_T = 12$ points along the translated line C_T, convergence is satisfactory, i.e. even with a total of only 300 two-particle states. We note that the experimental value for the width of the first excited $J^\pi = 2_1^+$ is $\Gamma \approx 113$ keV and that the energy is $\mathrm{Re}(E)_{2_1^+} = 1797$ keV. Our simplified nucleon–nucleon interaction gives a qualitative reproduction of the data. In addition we have neglected the contribution of $p_{1/2}$ single-particle motion, which would add more binding to the two-particle states of ^{6}He.

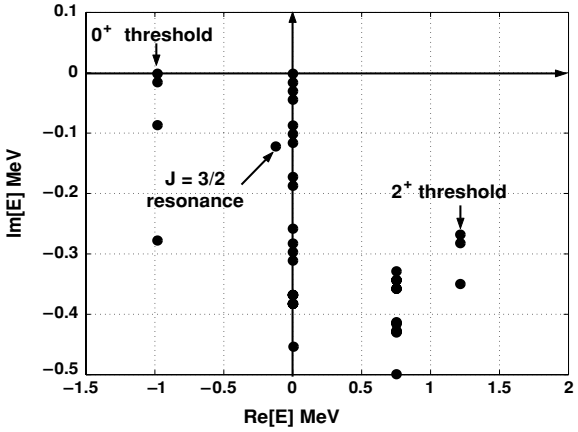

Figure 2. Plot of the $3/2^-$ complex energy spectrum of ^{7}He for a model space consisting of $p_{3/2}$ single-particle orbits only. The $J^\pi = 3/2^-$ resonance is located at $E_{3/2^-} = -(0.120\,731 + 0.122\,211\mathrm{i})$ MeV.

Table 2. Convergence of the 0^+ bound state and 2^+ resonant state energy in ^{6}He in terms of the number integration points N_R and N_T along the rotated C_R and the translated part C_T of the contour, respectively. The number N_{2p} gives the dimension of the two-particle anti-symmetrized basis. Here only $p_{3/2}$ single-particle orbits are included. Energies in MeV.

			0^+		2^+	
N_R	N_T	N_{2p}	Re(E)	Im(E)	Re(E)	Im(E)
12	12	300	−0.980 067	−0.000 759	1.215 956	−0.267 521
20	20	820	−0.979 508	0.000 000	1.216 495	−0.267 745
25	25	1275	−0.979 509	0.000 000	1.216 496	−0.267 745

Finally we consider the unbound nucleus ^{7}He, with ground state ($J^\pi = 3/2^-$) located $\approx$0.5 MeV above the ^{6}He ground state, and with a measured width $\Gamma \approx 160$ keV. Other continuum structures, with tentative spin assignments $J^\pi = 1/2^-$, and $J^\pi = 5/2^-$, have been observed (see, for example, [20] for an extensive review of the experimental situation). Limiting the attention to a model defined by the $p_{3/2}$ single-particle orbits only, it is clear that only a $J^\pi = 3/2^-$ resonance can appear for the ^{7}He nucleus.

In the case of 24 mesh points in momentum space for the $p_{3/2}$ single-particle quantum numbers lj, the total dimension d of the ($J^\pi = 3/2^-$) three-particle problem is $d = 9224$. If in addition, we were to include 24 single-particle momenta for the $p_{1/2}$ single-particle quantum numbers lj, we would have roughly $d \sim 40\,000$ three-body configurations.

Figure 2 gives the energy spectrum after a full diagonalization of the three-particle GSM equation. It is seen that the choice of contour in calculating the single-particle spectrum is optimal in the sense that all physical interesting states are well separated from the dense distribution of complex scattering states. The $J^\pi = 3/2^-$ resonance appears at the energy $E_{3/2^-} = -(0.12 + 0.12i)$ MeV. The $J^\pi = 3/2^-$ energy spectrum of ^{7}He plotted in figure 2, shows that the 0^+ and 2^+ states in ^{6}He, and the $3/2^-$ state in ^{5}He, form complex thresholds. The physical interpretation of these three-particle states is, in the case of the ^{6}He thresholds, that two of the neutrons form either the 0^+ ground state or the 2^+ resonant state, while the third neutron is moving in a complex continuum orbit. In the case of the ^{5}He complex threshold, two neutrons move in complex-continuum orbits while the third forms the $3/2^-$ ground state in ^{5}He.

Table 3. Expansion coefficients of the $J^\pi = 3/2^-$ ground state in ^{7}He. Here only $p_{3/2}$ single-particle orbits are included.

	$\|p^3_{3/2}\rangle$	
	Re[C^2]	Im[C^2]
$\|RRR\rangle$	1.295 549	−0.986 836
$\|RRC\rangle$	−0.184 544	1.099 729
$\|RCC\rangle$	−0.115 738	−0.110 375
$\|CCC\rangle$	0.004 733	−0.002 518

A diagonalization within the reduced space, where at most two particles move in continuum orbits, gives the resonance energy $-(0.14 + 0.16\text{i})$ MeV, which shows that the effect coming from all particles moving in the continuum is not negligible, but small.

Table 3 gives the squared amplitudes of the various single-particle configurations in the ^{7}He ground state, $\{|RRR\rangle, |RRC\rangle, |RCC\rangle, |CCC\rangle\}$, where R labels a single-particle resonance and C a complex single-particle continuum orbit. It is seen that the most important configuration is that where all single-particles are in the $p_{3/2}$ single-particle resonant orbit, as expected. The effect of configurations where all particles are in continuum orbits is small, which suggest that the coupling to configurations $|CCC\rangle$ may be taken into account perturbatively (see [21]).

In figure 2 we note that the $J^\pi = 3/2^-$ ground state in ^{7}He appears at an energy of approximately 0.86 MeV above the ground state in ^{6}He, while the experimental value is at approximately 0.5 MeV. This discrepancy with experiment can be understood by expanding the main component of the wavefunction, $|RRR\rangle$, in coefficients of fractional parentage. From the geometry it is found that the configuration where two of the particles are coupled to $J = 2$ has an amplitude of $\sqrt{5/6}$ while the configuration where the two particles are coupled to $J = 0$ has an amplitude of $\sqrt{1/6}$. In our calculations the 2^+_1 resonance comes at an energy $\approx(1.2 - 0.26\text{i})$ MeV, which is roughly 2.2 MeV above the 0^+_1 ground state of ^{6}He, to be contrasted with the experimental value of $\approx$1.8 MeV. This suggests that if we were to increase the attractive strength of the $J^\pi = 2^+$ interaction in ^{6}He and get a better agreement with the experimental value, the $J^\pi = 3/2^-$ resonant ground state of ^{7}He would also get closer to the experimental results.

2. Effective interactions for gamow shell-model calculations

The previous section served to introduce and motivate the application of complex scaling and a Berggren basis in studies of weakly bound nuclear systems. However, employing such a momentum space basis soon exceeds feasible dimensionalities in SM studies. To circumvent this problem and to be able to define effective interactions of practical use in SM calculations, we introduce effective two-body interactions based on similarity transformation methods. These interactions are in turn employed in GSM calculations. We base our approach on the extensive works of Suzuki, Okamoto, Lee and collaborators (see, for example, [23–26]). This similarity transformation method has been widely used in the construction of effective two- and three-body interactions for use in the No-Core SM approach of Barrett, Navratil, Vary and collaborators (see, for example, [27–30] and references therein). However, since the similarity transformation method has previously only been considered for real interactions, we need to extend its use to GSM calculations, implying a generalization to complex interactions.

To achieve the latter we introduce first the SM secular equation for two valence particles,

$$H\left|\Psi_\alpha^J\right\rangle = (H_0 + V_{12})\left|\Psi_\alpha^J\right\rangle = E_\alpha\left|\Psi_\alpha^J\right\rangle, \tag{2.1}$$

where H_0 includes the single-particle part of the Hamiltonian, kinetic energy and an eventual single-particle potential. The term V_{12} is the residual two-body interaction. The exact wavefunction Ψ_α^J is expanded in terms of two-particle Slater determinants, generated from the single-particle basis of H_0, corresponding to the basis from the ^{5}He calculations of subsection 1.1.

The aim is to construct an effective interaction in a reduced two-particle space (model space). Starting with the single-particle Berggren basis for ^{5}He, the space spanned by this basis is divided into a model space (p) and a corresponding complement space (q). These single-particle spaces define in turn our two- (and many-particle) model spaces

$$P = \sum_{a\leqslant b}\left|\Phi_{a,b}^J(1,2)\right\rangle\left\langle\tilde{\Phi}_{a,b}^J(1,2)\right|, \qquad a,b\in p \tag{2.2}$$

and the complement spaces

$$Q = \sum_{a\leqslant b}\left|\Phi_{a,b}^J(1,2)\right\rangle\left\langle\tilde{\Phi}_{a,b}^J(1,2)\right|, \qquad \begin{cases} a\in p \ \wedge\ b\in q \\ a,b\in q. \end{cases} \tag{2.3}$$

The projection operators fulfil the relations

$$P^2 = P, \qquad Q^2 = Q, \qquad P^{\mathrm{T}} = P, \tag{2.4}$$

and

$$Q^{\mathrm{T}} = Q, \qquad P + Q = 1, \qquad PQ = 0, \tag{2.5}$$

where T indicates the transpose. The first challenge is then obviously how to define a suitable single-particle model space within the Berggren formalism. Ideally the model space should consist of the single-particle orbitals which in the two-, three- and many-body problems give the most important many-body correlations. Dealing with a single-particle Berggren basis, selecting p is not a straightforward procedure. First, it is rather obvious that the single-particle resonant orbitals should be part of p, on the other hand it is not obvious which non-resonant continuum orbitals should be part of p. One could for example choose the continuum orbitals lowest in real, imaginary or absolute value of the energy, or should one rather choose the non-resonant continuum orbitals closest in energy to the single-particle resonances?

Our prescription for selecting p is based on our knowledge of the physical system, ^{7}He, in which we wish to apply the effective two-body interaction. In section 1 it was pointed out that the $J^\pi = 3/2^-$ ground state of ^{7}He has the 2^+ resonance in ^{6}He as an important two-body configuration. Based on this result, a viable starting point is to study the single-particle strengths in the 2^+ resonance wavefunction. Thereafter we define a single-particle model space consisting of those resonant and complex continuum orbitals having the largest absolute value of the single-particle strength. With this recipe we have a consistent way of defining a single-particle model space, which forms the basis for constructing an effective interaction in the two-particle model space.

Having defined a two-particle model space, we wish to construct an effective two-body interaction within p, which reproduces in the p-space exactly N_P selected eigenvalues of the full Hamiltonian. This can be accomplished by a similarity transformation

$$\tilde{H} = \mathrm{e}^{-\omega} H\,\mathrm{e}^{\omega}, \tag{2.6}$$

where ω is defined by $\omega = Q\omega P$. It follows that $\omega^2 = \omega^3 = \cdots = 0$ and $\mathrm{e}^\omega = P + Q + \omega$. The two-body secular equation (2.1) is then rewritten in a 2×2-block structure. If $P\tilde{H}P$ is to be

the two-particle effective interaction, reproducing exactly N_P eigenvalues of H, the decoupling condition $P\tilde{H}Q = 0$ must be fulfilled. One may show that the decoupling condition becomes [23, 24]

$$QHP + QHQ\omega - \omega PHP - \omega PHQ\omega = 0, \tag{2.7}$$

with ω acting as a transformation from the model space p to its complement Q, namely,

$$\left\langle \tilde{\Phi}^J_{c,d} \middle| \Psi^J_\alpha \right\rangle = \sum_{a \leqslant b} \left\langle \tilde{\Phi}^J_{c,d} \middle| \omega \middle| \Phi^J_{a,b} \right\rangle \left\langle \tilde{\Phi}^J_{a,b} \middle| \Psi^J_\alpha \right\rangle, \tag{2.8}$$

where $\Phi^J_{a,b} \in P$ and $\Phi^J_{c,d} \in Q$ respectively. In constructing the two-body effective interaction, one obviously needs the solution for the transformation operator ω. This is obtained in two-steps. In the first step the two-body secular equation (2.1) is solved exactly, this is done for ^{6}He in subsection 1.2 for all relevant spins. Secondly, N_P exact solutions of equation (2.1) are selected, and this set of exact solutions then enters equation (2.8). Now the question arises which N_P exact solutions should be picked out. The effective interaction generated in the model space depends on the N_P exact solutions entering equation (2.8). This is why the effective interaction generated by the similarity transformation method is often called *State-Dependent effective interaction*. There is no unique solution for ω. From equation (2.8), it is seen that the solution for ω may be obtained as long as the matrix $\left\langle \tilde{\Phi}^J_{a,b} \middle| \Psi^J_\alpha \right\rangle$ is invertible and non-singular. On the basis of this, we choose those N_P exact solutions Ψ^J_α with the largest overlap with the two-particle model space states $\Phi^J_{a,b}$. With the solution ω, the non-Hermitian effective interaction R is given by [23, 24]

$$R = P\tilde{H}P - PH_0P = PV_{12}P + PV_{12}Q\omega. \tag{2.9}$$

It would be preferable to obtain a complex symmetric effective interaction, in order to take advantage of the anti symmetrization of the two-particle basis. This may be accomplished by a complex orthogonal transformation

$$V_{\text{eff}} = U^{-1}(H_0 + V_{12})U - H_0, \tag{2.10}$$

where U is complex orthogonal and defined by

$$U = \exp(-S), \qquad S = \operatorname{arctanh}(\omega - \omega^T). \tag{2.11}$$

Such complex orthogonal transformations preserve the Berggren metric $x^T x$ of any vector $x \in \{C^n\}$. This feature allows us to define a complex symmetric effective two-body interaction

$$V_{\text{eff}} = (P + \omega^{\mathrm{T}}\omega)^{1/2}(PHP + PHQ\omega)(P + \omega^{\mathrm{T}}\omega)^{-1/2} - H_0. \tag{2.12}$$

In the limit $N_P = N$, where N is dimension of the complete two-body problem, the effective interaction equals the 'bare' interaction (V_{12}). To determine V_{eff} numerically, one has to find the square root of the matrix $A = (P + \omega^{\mathrm{T}}\omega)$. It can be shown that the square root of the matrix is related to the matrix sign function (see [31] for more details). An approach suitable for complex matrices is based on iterations of the matrix sign function (see [32]).

Below we apply the Lee–Suzuki similarity transformation method to the GSM calculation of the ground state of ^{7}He, for the case of $p_{3/2}$ single-particle motion only, fully diagonalized in subsection 1.2.

Figures 3 and 4 show the convergence of the real and imaginary part of the $J^\pi = 3/2^-$ resonance in ^{7}He, as the model space is increased. For comparison we plot the results for a diagonalization within the model space using the 'bare' interaction. It is seen that the results with the effective interaction constructed with the similarity transformation method converges much faster than the results obtained with the 'bare' interaction. We see that a satisfactory convergence is obtained with 10–11 single-particle Berggren states in the single-particle model

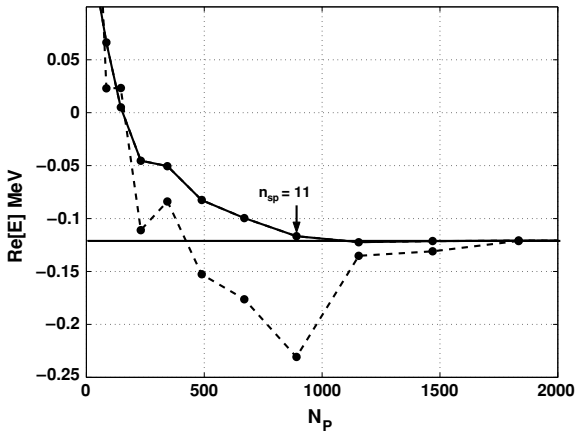

Figure 3. Convergence of the real part of the $J^\pi = 3/2^-$ resonance in ^{7}He for a space defined by occupation of $p_{3/2}$ single-particle orbits only. The abscissa represents the number of three-particle model space configurations N_P while $n_{\rm sp}$ represents the total number of single-particle momenta for the $p_{3/2}$ single-particle quantum numbers lj. The solid line corresponds to the effective interaction generated by the Lee–Suzuki similarity transformation method, while the dashed line is obtained using the bare interaction and the same number of three-body configurations. The $3/2^-$ resonance is located at $E = -(0.120\,731 + 0.122\,211\mathrm{i})$ MeV. The horizontal line is the real energy obtained in the full space of three-body configurations.

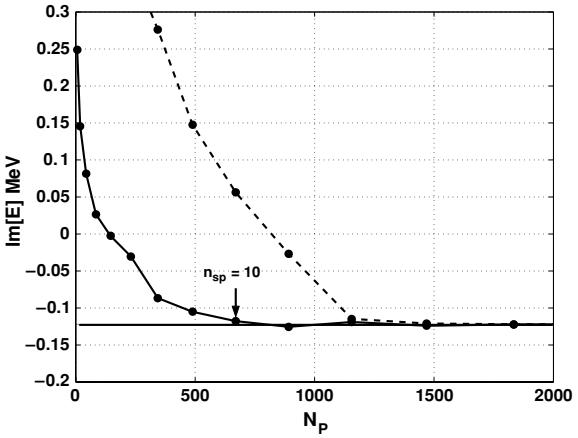

Figure 4. Same legend as in figure 3, but now for the imaginary part.

space p from ^{5}He, corresponding to ≈700–800 three-particle states N_P. Compared with the full dimension of the three-particle problem, 9224, we have drastically reduced the dimension to about 8% of the full space. This is a considerable benefit which may allow us to extend the GSM with a complex scaled single-particle basis to heavier systems and realistic effective interactions.

3. Conclusion and future perspectives

The main topic in this paper has been to present an algorithm for GSM calculations for nuclei with more than two active particles. Our emphasis is on the derivation of effective interactions

for such systems. We demonstrated that the construction of an effective two-body interaction based on the Lee–Suzuki similarity transformation method, leads to a drastic reduction of the GSM dimensionality for more than two particles. This result is promising when extending the GSM to applications in structure calculations of heavier dripline nuclei, with a larger number of valence particles moving in a large valence space.

With further progress in computational power one may hope that *ab initio* calculations of light and medium size nuclei within the Berggren representation may become possible in the near future. Coupled-cluster techniques have proven to be a promising method for calculations of medium size nuclei. Very recently [33–35], converged coupled-cluster results for the ground- and first excited state of ^{16}O where reported, using modern nucleon–nucleon interactions derived from effective field theory. A promising way of approach would be to generalize the coupled-cluster method to complex interactions, and at the first stage see how resonant structures are formed in light nuclei starting from an *ab initio* approach. Another interesting application would be to see how single-particle resonances are formed starting from a realistic nucleon–nucleon interaction.

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