Description of resonances in light nuclei using a microscopic cluster model

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Abstract

We investigate resonances in light halo nuclei using a fully microscopic cluster model and the complex scaling method. We make use of the hermitian representation of the complex scaling method. The general structure of the cluster model is that of a correlation operator acting on a starting function that describes a number of neutrons relative to an alpha-particle. The correlation operator is expanded in terms of a small non-orthogonal set of Gaussian basis states and we make use of a simplified, central but state-dependent, interaction. The many-body integrals required for the computation are evaluated by a variational Monte-Carlo algorithm. We show how to obtain resonant states for both $^5$He and $^6$He.

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The study of resonant structures in loosely bound systems, such as halo nuclei, is an interesting area of nuclear physics that promises to be a rich source of information on many-body dynamics. There exists a variety of methods for analyzing such structures and in this work we consider an approach that belongs to the category of cluster models, which have proven to be powerful tools in analyzing the structure of such loosely bound systems. The most common way in which present cluster models describe the continuum structure of light nuclei is by treating only the most important degrees of freedom properly, and ignore the difficulties with the Pauli principle that entails. In contrast to such approaches, we employ a fully microscopic cluster model in order to provide a variational approximation to the Schrödinger equation with, in this case, a slightly simplified nucleon-nucleon interaction.

A related microscopic cluster model that can deal with three-body resonances by complex-scaling in coordinate space was developed by Csoto and applied to $^6$He, $^6$Li and $^6$Be [1]. This model can account in many cases both for the correct nuclear physics and proper three-body dynamics. Among other results the authors predict the non-existence of the soft dipole resonance in $^6$He. Another example of a similar study of halo nuclei by the complex scaling method through a microscopic model can be found in Ref. [2]. An alternative to the use of the complex scaling in coordinate space is to perform a contour deformation in momentum space [3]. This was applied at the level of a two-body problem and an extension to few-body Borromean halo systems is in progress.

Despite the success of the two- and three-body microscopic cluster models the existing fully microscopic ones have problems when considering resonances [4]. The ab-initio approaches, e.g., the Monte-Carlo approach of Ref. [5], even though very well suited for the bound-state problem, have difficulties describing resonances.

By using the complex scaling method [6, 7] in the ‘direct approach’, our model can handle resonances correctly in a straightforward way. The wavefunction we employ is fully microscopic and is explicitly antisymmetrized so that the Pauli exclusion principle is exactly satisfied. The general structure is that of a correlation operator acting on a reference function that describes a number of neutrons relative to an alpha-particle. We include a multiplicative Jastrow factor for the short-range correlations and an additive configuration-interaction (CI) term for the long-range correlations. This last term only introduces pair correlations, whereas the Jastrow term also includes higher correlations. This mechanism has proved to be efficient in describing nuclear structure in various applications to closed and open shell
systems, where all particles are treated on an equal footing \cite{8,9}. Recently, this has also been applied \cite{10} to nuclei with $12 \leq A \leq 16$.

One advantage of the Jastrow-CI scheme is the explicit inclusion of translational invariance and the fact that the correlation operators can be sufficiently well approximated by a small non-orthogonal basis set that makes application to heavier nuclei possible. For the moment we confine ourselves to central $V_4$ interactions and in particular we make use of the S3 interaction of Afnan and Tang \cite{11}. For the computation of the many-body matrix elements we make use of the Variational Monte Carlo method, which we have analyzed in detail \cite{12} as applied to this cluster model.

In this letter we focus on the cases of $^5$He and $^6$He. Although experimentally $^5$He is unbound while $^6$He is lightly bound, the absence of spin-orbit force in our simplified force results in both nuclei being unbound. Nevertheless, both nuclei exhibit a rich resonance structure. The current work thus provides an excellent testing ground for the study of resonances, even though the nuclear physics may not be wholly realistic.

There exists many different version of the complex scaling technique. In the original complex-coordinate method (see, e.g., Ref. \cite{6}) the resonance position $E_R$ and width $\Gamma$ are calculated from the complex eigenvalue $E = E_R - i\Gamma/2$ of a non-hermitian Hamiltonian. The non-hermitian Hamiltonian is obtained from the original one by a transformation of the particle coordinates. Here we shall only use the most straightforward one, $r \to r \exp(i\theta)$, where the angle $\theta$ is the scaling parameter. Such a transformation leaves the bound states unaffected and rotates the positive energy scattering states by an angle of $2\theta$ into the lower part of the complex plane relative to the threshold \cite{6,7}. Resonant states $\Psi_{\text{res}}$ appear as complex eigenvalues in the lower half complex plane that are invariant with respect to changes in the scaling parameter $\theta$, as long as this angle is large enough to uncover the resonances. [A more detailed review of the complex scaling method can be found in \cite{7}.]

For a complex scaled Hamiltonian, the complex variational principle, unlike the conventional one, is a stationary principle rather than a minimum principle for either the resonance position or width. This is not very attractive, and Moiseyev \cite{13} has formulated a representation of the complex-coordinate method in which the resonance position $E_r$ and width $-2E_i$ are variational parameters of a hermitian Hamiltonian which gives additional stability, especially when working with small basis sets, as in this work. It is also gives a simple algorithm to follow the path of a given eigenvalue as $\theta$ changes. The variational method was
reformulated by Bylicki [14], into a simpler and more convenient form.

In this method, we first rewrite the complex scaled Schrödinger equation as

\[
(\hat{H}_r + i\hat{H}_i)(\Psi_r + i\Psi_i) = (E_r + iE_i)(\Psi_r + i\Psi_i),
\]

(1)

where \( \hat{H}_r \) and \( \hat{H}_i \) are the real and imaginary parts of the scaled Hamiltonian \( \hat{H}(re^{i\theta}) \). In matrix form this becomes

\[
\mathcal{H}(E)\Psi = 0, \quad \mathcal{H} = \begin{pmatrix}
-\hat{H}_i + E_i & \hat{H}_r - E_r \\
\hat{H}_r - E_r & \hat{H}_i - E_i
\end{pmatrix}, \quad \Psi = \begin{pmatrix}
\Psi_i \\
\Psi_r
\end{pmatrix}.
\]

(2)

Since the exact eigenvalue of \( \hat{H}(re^{i\theta}) \) is unknown we can consider the alternative equation

\[
\mathcal{H}(E)\Phi = \lambda\Phi,
\]

(3)

where \( \Phi \) is an approximation to the exact wavefunction \( \Psi \). For a particular value of the scaling parameter \( \theta \) the best choice of \( \Phi \) is obtained by minimizing the size of \( \lambda \), and \( \Phi = \Psi \) if \( \lambda = 0 \). Within this approximation the parameters \( E_r \) and \( E_i \) that appear in \( \mathcal{H} \) no longer represent the exact real and imaginary parts of the complex energy but become variational parameters. Thus in addition to the linear variational principle that is employed for the wavefunction we also have to vary \( E_r \) and \( E_i \) so as to minimize \(|\lambda|\). Although \( \lambda \) has both positive and negative values one interesting property of Eq. (2) is that the spectrum of eigenvalues is symmetric around 0, thus if \(|\lambda|\) is an eigenvalue so is \(-|\lambda|\).

Furthermore, the equation \( \mathcal{H}^2\Phi = \lambda^2\Phi \) is useful for obtaining bounds for the resonance position and width and it can be used in an iterative method for determining the values of \( E_r \) and \( E_i \) that minimize \(|\lambda|\).

The many body Hamiltonian is of the form

\[
\hat{H} = \sum_{i=1}^{A} \frac{\hbar^2}{2m_i} \nabla_i^2 + \sum_{1\leq i<j}^{A} V(ij),
\]

(4)

In this letter, we use a semi-realistic central nucleon-nucleon interaction (V4) interaction that has the general form

\[
V(ij) = V_0(ij) + V_\sigma(ij) + V_r(ij) + V_{\sigma\tau}(ij).
\]

(5)

Here the \( V_{\sigma/r} \) are the spin/isospin-dependent part composed of spin/isospin-exchange operators. The radial part of each channel potential is expanded as a sum of Gaussian functions. We use the S3 interaction of Afnan and Tang [11].
For the trial wavefunction we consider the linearized approximation of the many-body wavefunction in terms of correlation operators acting on an uncorrelated reference function [15]. This provides a translationally invariant description of the many-body problem and was applied to a number of closed-shell systems in terms of an alpha-cluster model [16]. The wavefunction $\Psi$ is given by $\Psi = \hat{F}\Phi_0$, where $\Phi_0$ is the reference function, that we take to be the product of the different cluster wavefunctions. The correlation operator $\hat{F}$ is of the form

$$\hat{F} = \sum_{k=1}^{N} \hat{F}_k \left( \sum_{k=1}^{N} a_k \sum_{i<j} f^k(ij) \right) \prod_{i<j} g(ij),$$  \hspace{1cm} (6)

$$f(ij) = \exp(dkr_{ij}^2), \quad g(ij) = 1 - k_1 \exp(-\lambda_1 r_{ij}^2) - k_2 \exp(-\lambda_2 r_{ij}^2).$$  \hspace{1cm} (7)

This type of wavefunction (referred to as the J-TICI(2) scheme) has been extensively used for the alpha-particle [8, 9] where it was shown to provide an adequate description for the ground-state properties. An important aspect of this approximation is the expansion of the correlation operator in terms of the non-orthogonal Gaussian functions $\exp(dkr_{ij}^2)$. Only a very small number of components is required for a reasonable convergence, something that makes calculations in the J-TICI(2) scheme less expensive than other microscopic methods.

Due to the complexity of the correlation operator we can make use of the variational Monte Carlo method for the evaluation of the matrix elements, where the probability density function $w$ is taken to be the square of one of the components in the expansion of the wavefunction, i.e., $w = (\hat{F}_0\Phi_0)^2$. This is a natural choice for the PDF since the wavefunction can always be written as the product of $w$ and a function $\Psi'$. This is discussed in detail in Ref. [12].

Thus Eq. (1) is approximated in terms of a non-orthogonal expansion. The non-orthogonality requires that in Eq. (2) the real and imaginary parts of the complex scaled Hamiltonian are modified according to

$$\hat{H}_r \rightarrow N^{-1/2} \hat{H}_r N^{-1/2}, \quad \hat{H}_i \rightarrow N^{-1/2} \hat{H}_i N^{-1/2}.$$  \hspace{1cm} (8)

$N$ represents the overlap matrix and $N^{-1/2} = CA^{-1/2}C^{-1}$, where $C$ is the matrix with the eigenvectors of $N$ as its columns and $A$ is the diagonal matrix with the eigenvalues of $N$ as its elements.

We firstly examine the application of the formalism of Moiseyev and Bylicki to the alpha-particle, where we do not expect to find any resonances. For the alpha-particle reference
function we use the spherically symmetric harmonic oscillator ground state. It is an easy numerical calculation both in terms of computation time and complexity. We can go one step further by introducing one or two additional nucleons, corresponding to the cases of $^5\text{He}$ and $^6\text{He}$.

Experimentally the alpha-particle is a stable nucleus with 20 MeV difference between the ground and first excited state. Searching for resonances is thus not extremely important, but the calculation will help to highlight the implications of the approximation scheme used. The results are displayed in Fig. 1. The threshold for this calculation is the ground state energy as obtained from the variational approximation ($\approx -27.3$ MeV). As can be seen from Fig. 1 the ground-state remains almost constant for small $\theta$ but when we increase $\theta$ further it eventually moves. This is not unexpected since the variational ground state is only an approximation to the exact threshold and it has a non-zero overlap with continuum states. It also suggests that we should optimize our basis to change with $\theta$—in this context we are especially concerned about the Jastrow factor. The rest of the eigenvalues move clockwise into the lower complex plane, eventually turning up as well. The behaviour of the threshold is somewhat of a worry, and shows that our variational form is not too good for finite $\theta$. 

FIG. 1: $\theta$-trajectories for the spectrum of the alpha-particle for various values of the rotation parameter $\theta$ between 0 and 0.65 radians. The value of the ground state corresponding to $\theta = 0$ is -27.3 MeV. The threshold is not stationary but rotates into the upper quadrant of the complex plain, while the rest of the eigenvalues move clockwise into the lower complex plain.
FIG. 2: θ-trajectories obtained for $^5\text{He}$ $L = 1$ ($J^\pi = 1/2^-, 3/2^-$) for various values of the width parameter $w$. In each plot the rotation parameter $\theta$ is varied in equal steps and the θ-trajectories evolve from right to left as $\theta$ is increased.

In all likelihood this is caused by the Gaussian functions in the Jastrow correlations (i.e., the short range behaviour of the wave function), but this requires confirmation. Clearly, we expect all calculations to fail for $\theta = \pi/4$, where all Gaussians become oscillatory.

Experimentally $^5\text{He}$ is unbound by 0.798 MeV and is observed as a $J^\pi = 3/2^-; T = 1/2$ resonance in the neutron scattering on $^4\text{He}$. In our approximation the case of $^5\text{He}$ is that where a neutron is added to the alpha particle wavefunction, where the additional coordinates are specified relative to the alpha-particle center-of-mass. The additional neutron is placed within a spherical shell and the many-body wavefunction has the form

$$\Psi_{^5\text{He}} = \hat{F}_A (\Phi_\alpha f(r_{a5}) \mathcal{Y}_M^L (r_{a5}) \times \chi_{\sigma \tau} (S, T)), \quad (9)$$

$$f(r_{a5}) = \exp \left( - \left( \frac{r_{a5} - d}{w} \right)^2 \right), \quad (10)$$

where $\mathcal{Y}_M^L (r_{a5})$ is a solid harmonic, while $\chi_{\sigma \tau} (S, T)$ represents the spin and isospin degrees of freedom. In the function $f(r_{a5})$ the parameter $d$ represents the distance from the alpha-particle, while $w$ represents the width of the shell. $r_{a5}$ is the relative distance of the neutron from the alpha-particle. The linear correlation operator is invariant under permutation of particle labels and can be taken outside the antisymmetrizer.

Both $d$ and $w$ are variational parameters and in principle we can have a number of them, i.e. expand over a number of shells each placed at a different distance from the alpha-particle with a given width. However, as $w$ increases the value of $d$ becomes insignificant and we
can consider a single shell provided \( w \) is large enough. The results obtained for \( L = 1 \) \((J^\pi = 1/2^-, 3/2^-)\) are illustrated in Fig. 2, where we have plotted \( \theta \)-trajectories for various values of the variational parameter \( w \). For relatively small values of \( w \) the trajectory is a smooth curve. As \( w \) is increased this curve gains a turning point that eventually becomes a cusp (left-hand part of Fig. 2). Further increase of \( \theta \) leads to loop-like trajectories (right-hand part of the figure).

In order to find the best \( \theta \)-trajectory we refer to the derivative of the eigenvalue with respect to \( \theta \). At resonance we expect that the energy is stable with respect to \( \theta \), i.e. \( \frac{dE}{d\theta} = 0 \). Thus the best \( w \) is that where \( \frac{dE}{d\theta} \) is closest to zero. This is illustrated in Fig. 3, where we can see the minimum value of \( |\Delta E| \) of the \( \theta \)-trajectory (corresponding to the absolute distance between two adjacent points) for a particular value of \( w \). The presence of a resonance is observed as the minimum value of \( |\Delta E| \) that occurs in a range of \( w \) between 5 and 6. According to Fig. 2 this corresponds to a cusp in the trajectory. The threshold for the problem (which is not shown in this figure) follows the trajectory for the \(^4\text{He}\) ground state, as shown Fig. 1 closely. This suggests little influence from the halo structure, on this state, and little influence from this state on the continuous spectrum of \(^5\text{He}\). From the obtained \( \theta \)-trajectories we can infer a complex eigenvalue corresponding to a resonance in the region \((E_r = -26 \pm 0.5 \text{ MeV}, E_i = -23.2 \pm 0.5 \text{ MeV})\), for \( \theta = 0.35 \). At this point the real part of the threshold has moved, but it has not developed an appreciable imaginary part. This
movement means that the threshold subtraction is somewhat uncertain. Nevertheless, it seems most sensible to use the $\theta = 0$ $^4\text{He}$ binding energy as threshold, $-27.3$ MeV. We thus find that a resonance $1.3\pm0.5$ MeV above threshold with a width of $2E_i = -46.4 \pm 1$ MeV. The uncertainty arising from the anomalous movement of the threshold with $\theta$ is unknown, but as argued above probably small.

Having ensured the applicability of the complex-scaling method to $^5\text{He}$ we proceed to the case of $^6\text{He}$. In the case of $^6\text{He}$ we experimentally have a Borromean nucleus: while $^5\text{He}$ is unbound, the $^6\text{He}$ ground state is stable. This state lies only $0.973$ MeV below the threshold for decay into an alpha-particle and two neutrons ($^4\text{He} + 2\text{n}$) and thus $^6\text{He}$ is very weakly bound. The first resonance of $^6\text{He}$ ($J^\pi = 2^+$) lies $1.797$ MeV above the ground state and has a strong decay to the $^4\text{He} + 2\text{n}$ channel. We find no bound states in our calculation due to the lack of spin-orbit force in the simplified nucleon-nucleon interaction used. However, we can examine the structure of low-energy resonances in this light nucleus. In our model $^6\text{He}$ is described by two neutrons added to the alpha particle wavefunction, where the additional coordinates are specified relative to the alpha-particle center-of-mass. Similar to the case of $^5\text{He}$ the two-neutrons are placed within a spherical shell, each parameterized in terms of a shifted Gaussian with an additional term describing the interaction of the two neutrons. This leads to a reference function, $\Phi_0$, that has the form

$$\Phi_0 = A\{\Phi_\alpha Y^L_{r_{a5}, r_{a6}} \exp \left( -\frac{(r_{a5} - d_{55})^2}{w_5} \right) \exp \left( -\frac{(r_{a6} - d_{66})^2}{w_6} \right) \exp \left( -\frac{(r_{56} - d_{56})^2}{w_{56}} \right) \},$$

where $r_{ai}$ is the relative distance of the $i$th neutron from the alpha-particle, while $r_{56}$ is the relative distance between the two neutrons. $Y^L_{r_{a5}, r_{a6}}$ is a solid harmonic that couples the two neutrons relative to the alpha particle to a total orbital momentum $L$.

The calculation is considerably more difficult than that of $^5\text{He}$, because of the increase both in configuration space and in the number of variational parameters. However, it is sufficient to consider a restricted set of variational parameters for a qualitative understanding. The results obtained look rather similar to those of $^5\text{He}$. In Fig. 4, the separation between the alpha-particle and the dineutron center-of-mass is kept fixed, while the the separation of the two-neutrons, represented by $w$, is varied. For small values of $w$ the $\theta$-trajectories are smooth curves, while a cusp is observed when $w$ is sufficiently large. Again, this eventually changes into a loop.
FIG. 4: The results obtained for $^6$He $L = 0$ ($J^\pi = 0^+$) for various values of the width parameter $w$. In this case $w$ is related to the separation of the two neutrons that are placed in a shell around the alpha-particle. In each plot the rotation parameter $\theta$ is varied in equal steps and the $\theta$-trajectories evolve from right to left.

Despite the qualitative nature of the results a clear resonant structure is obtained. In both $^5$He and $^6$He calculations only 9 components are used for the expansion of the correlation operator, and this is enough for providing convergence. The small basis set allows the calculations to be carried without any significant restrictions in the numerical method. The only difficulty that arises in going to heavier systems will be due to the explicit antisymmetrization. As a result of the hermitian representation of the complex variational principle is simple to obtain $\theta$-trajectories for the complex eigenvalues. In order to identify the resonance we use the condition that at resonance the complex energy should be stationary with respect to the scaling parameter. For the moment the results obtained are somewhat qualitative. Although the numerical error due to the Monte-Carlo sampling is trivial for a particular point in the $\theta$-trajectories, the optimal value of the variational parameters (e.g. $w$) that gives the resonance could only be obtained within a range. Precise determination of that would require a much more elaborate calculation.

Another point that needs further investigation is the fact that the basis set employed does not provide a fixed threshold for the alpha-particle. It is expected that this will further influence the position of the resonance but is not clear at this stage in exactly what way. Nevertheless, the difference between the $\theta$-trajectories for the alpha-particle and those of $^5$He and $^6$He is quite profound. The position where the resonance occurs for both $^5$He and $^6$He is
at a point where the motion of the alpha-particle continuum due to the scaling is clockwise into the lower complex plain. Therefore, it is extremely unlikely that the resonance can be attributed to the anomalous behavior of the alpha-particle threshold.

We have examined the application of a fully microscopic cluster model to resonances in halo nuclei. We have obtained low-lying resonances for both $^5$He and $^6$He by determining the point where the complex energy is stationary with respect to a scaling parameter. This is encouraging since experimentally it is expected that both systems have low-lying resonances.

The central outcome of our investigation is that the complex-scaling method can be successfully applied to our fully microscopic model for weakly bound nuclei. This was achieved with a relatively simple approximation, where the number of basis functions is quite small. Within our framework of a non-orthogonal expansion it is convenient to make use of the variational Eq. (2), rather than the standard complex variational principle. Although both methods give the same results, the hermitian representation provides a systematic way of obtaining individual $\theta$-trajectories.

Apart from resonances our method provides an interesting way to investigate the correlation mechanism used, which is widely applied (Jastrow-CI). Despite the fact that such a correlation mechanism gives a good description of the bound-state properties of the alpha-particle, the ground state is not stationary under complex scaling. This suggests that the basis used to expand the correlation mechanism can be improved.

It is possible to obtain more accurate positions for these resonances and in the future we plan to improve and extend the calculation in order to get results of a more quantitative nature. This would include both increasing the accuracy (more computer time), and obtaining upper and lower bounds (as suggested in [4, 13]).

In this paper we are only interested in a qualitative understanding of the method. However, a more complete interaction can be used, which should lead to results comparable to the experimental data. Hence, the first natural step in extending the above work is to include a spin-orbit force in the nucleon-nucleon interaction. It is expected that this will be adequate to produce a bound state for $^6$He and at the same time allow the results for resonances to be of a more quantitative nature.
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