From nuclear structure to reactions with a unified continuum shell model approach

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Abstract. Within a unified formalism the chain of helium isotopes linked by neutron decay reactions is explored from bound states to resonances and cross sections in continuum. Using this realistic example the Continuum Shell Model formalism is presented and discussed.

1. Introduction
The description of a nuclear many-body problem that seamlessly traverses from structure to reactions is a central challenge for modern nuclear theory. The advent of new experimental radioactive beam techniques leading to rapid exploration of the nuclear chart; enormous advances in astrophysics along with realization of the important role played by exotic nuclei in reaction chains of stellar evolution and early universe; exploration of other mesoscopic many-body systems from quantum wires and dots to pentaquarks - all hinge on a good theoretical understanding of a quantum many-body system that is coupled to a continuum of external states.

The many-body problems on the border of structure and reactions have been extensively discussed in the past. The list of works extends from classical papers by Wigner, Feshbach, Weidenmüller and others [1, 2, 3] to the latest works such as found in Ref. [4, 5, 6]. In this paper we discuss a particular Continuum Shell Model (CoSMo) approach, further in-depth information can be found in [7]. We structure the presentation starting with the CoSMo result for the chain of helium isotopes shown in Fig. 1. The reader is urged to review this figure as the features of the model are being introduced and discussed in the following sections. The set of important points is highlighted through the text.

2. Traditional Shell Model and Beyond
The success of the traditional shell model (SM) [8] in the treatment of a nuclear many-body problem is unquestionable. In the SM the valence space appropriate for a problem is selected by defining a set of bound single particle (s.p.) states in the average nuclear mean filed. The many-body problem is solved by diagonalizing a Hamiltonian on the Slater determinant many-body basis states. Although SM has a rigorous theoretical footing practice shows that a very phenomenological attitude can be taken here: many questions about structure of nuclei can be answered without explicit discussion of the coordinate form of particle-particle interaction and without addressing an exact shape of the mean-field. The best example of this is a USD SM [8] where 3 s.p. energies in the sd shell along with 63 two-body matrix elements are simply considered as adjustable parameters and fitted to experiment. The resulting model
Figure 1. (Color online) CoSMo results for He isotopes. The states in the chain of isotopes starting from $^4\text{He}$ (top) to $^{10}\text{He}$ (bottom) are shown as a function of the energy relative to $^4\text{He}$. The horizontal dotted lines separate each isotope and for each case states from CoSMo are shown above experimentally observed states. The decay width (in MeV) is shown for each state along with spin and parity. The solid lines above CoSMo states show the elastic neutron scattering cross section from the spin polarized ground state of $N-1$ isotope. The construction of the model as well as the details of the calculation are discussed in the text that follows this figure.
is extremely successful in describing thousands of levels in $A=16$ to 40 mass nuclei. We refer to such Hamiltonian as $H_{SM}$.

In analogy to the SM the CoSMo approach defines the internal part of a full space with a set of Slater determinant states $|1\rangle$, where all $N$ nucleons are located on bound SM orbitals. In example of Fig. 1 the internal space contains two s.p. levels: $p_{1/2}$ and $p_{3/2}$. This traditional SM space is appended by the continuum of external reaction states $|c; E\rangle$, labeled here by the channel index $c$ and the running energy variable $E$. The reaction states are assumed to be energy normalized. Considering a full wave function as a superposition

$$|\alpha; E\rangle = \sum_1 \alpha_1(E)|1\rangle + \sum_c \int dE' \alpha_c(E'; E)|c; E'\rangle,$$  \hspace{1cm} (1)

the Schrödinger equation for the internal subspace becomes

$$\sum_2 \left[\langle 1|H|2\rangle + \sum_c \int dE' \frac{A_1^c(E', E)A_2^c(E', E)^*}{E - E' + i0} - \delta_{12}E\right] \alpha_2 = 0,$$  \hspace{1cm} (2)

where we introduced notations for the amplitude $A_1^c(E', E) = \langle 1|H - E|c; E'\rangle$ which defines the action of the Hamiltonian between internal and external spaces. The above form is particularly useful in establishing a correspondence with the traditional SM since Eq. (2) represents an eigenvalue problem with the non-Hermitian, energy-dependent effective Hamiltonian $[1, 3, 9, 7]$

$$\mathcal{H}(E) = H + \Delta(E) - \frac{i}{2} W(E), \quad \text{where}$$  \hspace{1cm} (3)

$$\langle 1|\Delta(E)|2\rangle = \sum_c \mathcal{P} \int dE' \frac{A_1^c(E', E')A_2^c(E', E')^*}{E - E'}, \quad \langle 1|W(E)|2\rangle = 2\pi \sum_c A_1^c(E)A_2^c(E)^*.$$  \hspace{1cm} (4)

The principal value term $\Delta$ is due to the off-shell processes of virtual excitation into external channel space, and the explicitly non-Hermitian term $W$ represents on-shell decays into the channels open at given energy, thus below all thresholds in stable states this term is identically zero. The traditional SM Hamiltonian can be identified as $H_{SM} = H + \Delta$ where energy dependence of self-energy term is ignored. We use this to define $H + \Delta$ within internal space to be $H_{SM}$. For the $^4\text{He}$ example the $H_{SM}$ is taken from old works $[10]$ the set of parameters contains 2 s.p. energies and 15 two-body matrix elements (only 7 $T = 1$ are relevant for $^4\text{He}$).

- By design of the CoSMo the energies of bound states coincide with the results of the traditional SM.

In Fig. 1 these are the nucleon-stable ground states of $^{4,6,8}\text{He}$. Departure from SM correspondence principle and inclusion of $\Delta(E)$ does not present any technical difficulty but this would require readjustment of SM interactions.

3. Continuum States and Decay Chains
The formulation (2) does not require external and internal spaces to be orthogonal; however the above form is valid only with the use of eigenchannels $H|c; E\rangle = E|c; E\rangle$ $[11]$. The general formalism can be found in $[1]$. We define continuum states as $|c; E_\alpha + \epsilon\rangle = b_\alpha^j(\epsilon)|\alpha; N - 1\rangle$ in the case of one particle in the continuum and $|c; E_\alpha + \epsilon + \epsilon'\rangle = b_\alpha^j(\epsilon)b_{\alpha'}^{j'}(\epsilon')|\alpha; N - 2\rangle$ for the two-nucleon continuum. Here $b_\alpha^j(\epsilon)$ is a s.p. creation operator of a continuum state at energy $\epsilon$ with quantum numbers $j$. We use realistically selected Woods-Saxon potential to define these states and thus identify Hamiltonian for the external space. The states $|\alpha; N - 1\rangle$ are eigenstates of an $N - 1$-body problem with energy $E_\alpha$. 
4. Decay Amplitudes and Thresholds

The on-shell amplitudes for a s.p. continuum channels are given as

\[ A_c^1(E) = a_j(\epsilon) \langle 1; N | b_j^\dagger | \alpha; N - 1 \rangle, \]  

where \( a_j(\epsilon) \) is a s.p. amplitude and the remaining terms in (5) represent a spectator wave function overlap. The s.p. decay width is related to the amplitude \( \gamma_j = 2\pi a_j^2 \). As discussed above the on-shell amplitudes are zero below thresholds. Assuming that the transition takes place from a SM internal s.p. state with radial wave function \( u_j(r) \) and is driven by a spherically symmetric nuclear potential \( V(r) \) (assumed also to be a Woods-Saxon in our example), the amplitude is

\[ a_j(\epsilon) = \sqrt{\frac{2}{\pi k_j}} \int_0^\infty dr F_l(k_j r) V(r) u_j(r), \quad \epsilon = \frac{k^2}{2\mu}, \]

where \( F_l \) is a regular solution of an asymptotic potential given by the Coulomb or Bessel function. As energy and corresponding momentum \( k \to 0 \) in the case of a neutral particle the energy dependence of an amplitude is determined by the asymptotic of the Bessel function leading to \( a_j(\epsilon) \propto \epsilon^{l/2 + 1/4} \) which gives correct kinematical properties of the two-body final state with a symmetry determined by the angular momentum \( l \). This kinematics permits phenomenological approach [7] where explicit form of the interaction \( V(r) \) and SM state \( u(r) \) is unnecessary, as the amplitude is parameterized using a single parameter \( a_j(\epsilon) = \kappa_j \epsilon^{l/2 + 1/4} \).

The two-body decay amplitudes can be divided into two types depending on the interaction that is responsible for such decays, see Fig. 2. The sequential decay represents a second order

\[ A_c^1(E) = \sum_\beta a_j(\epsilon) a_{j'}(\epsilon') \left( \frac{\langle 1 | b_j^\dagger | \beta \rangle \langle \beta | b_{j'}^\dagger | \alpha \rangle}{S_\beta + \epsilon} - \{\epsilon, j\} \leftrightarrow \{\epsilon', j'\} \right). \]

The process proceeds via all intermediate states \( \beta \) and is suppressed with a characteristic energy denominator involving a separation energy \( S_\beta \), see Fig. 2. In the case of a direct decay a nucleon pair is removed in a single step process, the resulting amplitude is

\[ A_c^1(E) = a^{(j_1 j_2)}(\epsilon_1, \epsilon_2) \langle 1; N | (p_{LL}^{j_1 j_2})^\dagger | \alpha; N - 2 \rangle, \]
where \( p^{(jj')}_{L} \) is a pair removal operator. The two-body removal amplitude \( a^{(j_1,j_2)}(\epsilon_1,\epsilon_2) \) can be computed with expression similar to (6), assuming that interaction between particles and the core is known. The kinematic energy-dependence of the two-body decay amplitudes at low energies is consistent with a three body final state phase space. In a fully symmetric case amplitude is directly proportional to the energy above threshold.

- The CoSMo approach includes a proper treatment of the near-threshold kinematics. The decay amplitudes and corresponding widths approach zero in accordance with the two or three body final state phase space volume.

5. Resonances

As mentioned the eigenvalue problem (2) \( H(E)|\alpha\rangle = E_\alpha |\alpha\rangle \) below thresholds is identical to the traditional SM. Above thresholds, however, the Eq. (2) has no real energy \( E = E_\alpha \) solutions because the boundary conditions set by internal and external problems can not be simultaneously satisfied at real energy. It is possible to remedy the situation and still use a discrete set of eigenvalues by defining resonances.

The Gamow definition analytically continues the energy into a complex plane \( E \rightarrow \mathcal{E} \) and the problem \( H(\mathcal{E})|\alpha\rangle = \mathcal{E}_\alpha |\alpha\rangle \) is then solved. The discrete set of solutions \( \mathcal{E}_\alpha \) represents a set of resonances with centroids \( E_r = \text{Re}\mathcal{E} \) and width \( \Gamma = -2\text{Im}\mathcal{E} \). As seen from Eq. (9) below, these solutions correspond to poles of scattering matrix. Although the Gamow definition is mathematically rigorous it requires a solution of the scattering problem at complex energy which is complicated and time consuming.

Breit-Wigner approach defines resonances via \( H(E)|\alpha\rangle = \mathcal{E}_\alpha |\alpha\rangle \) under condition \( E = \text{Re}\mathcal{E}_\alpha \). This approach avoids the need of reaction calculations at complex energies and it was used to obtain the discrete set of resonant states in Fig. 1. The problem is highly non-linear. Each resonant state is obtained in an iterative process where initial scattering energy \( E \) is taken from the traditional SM solution, then the non-Hermitian eigenvalue problem is solved leading to the complex eigenvalue, the real part of which is taken as a scattering energy for the next iteration.

We stress here several distinct features of resonances obtained in CoSMo:

- Both Hermitian and non-Hermitian parts of the Hamiltonian are diagonalized simultaneously, which fully takes into account all complicated diagrams involving internal states and continuum.
- Interference of decays and internal structure is accounted for.
- The structure of resonant states is affected by decays. The energies of states in Fig. 1 that are unstable (highlighted in red or with a lighter shade of gray) deviate from those given by SM. This is particularly important at strong continuum coupling when coherence with respect to decay leads to the super-radiance phenomenon [7, 12, 13].

6. Scattering Matrix and Unitarity

Unlike resonances the scattering cross section is an ultimate observable to be compared with experiment. As shown in [1] and discussed extensively in [7] the cross section in CoSMo is determined by the scattering matrix

\[
T^{cc'}(E) = \sum_{12} A^{c}_{1}(E) \left( \frac{1}{E - H(E)} \right)_{12} A^{c'}_{2}(E).
\]

Here the scattering process enters via channel \( c' \) given by amplitude \( A^{c'} \), propagates through internal system driven by the effective non-Hermitian operator \( H \) and exits via channel \( c \). The appearance of the full effective Hamiltonian in the above equation assures a proper treatment of the intermediate diagrams as well as the dissipation into other continuum channels. The
factorizable nature of \( W = 2\pi \mathbf{A} \mathbf{A}^\dagger \) in terms of channel matrix \( \mathbf{A} \) is crucial for the overall conservation of probability [14]. Through the use of the Dyson equation the unitarity of \( S\)-matrix can be explicitly shown [13],

\[
T = \frac{R}{1 + i\pi R}, \quad S = \frac{1 - i\pi R}{1 + i\pi R},
\]

where matrix \( R = \mathbf{A}^\dagger \frac{1}{E - H_{SM}} \mathbf{A} \) is introduced in analogy to the \( R\)-matrix of reaction theory.

In Fig. 1 the reaction cross sections are shown. They correspond to polarized neutrons scattering from the ground states of \( \text{He} \) nuclei in the chain.

- The cross sections include the loss of flux into all channels which is an essential part of the overall conservation of probability. The CoSMo \( S\)-matrix is unitary.
- Matrix inversion rather than diagonalization is involved in the cross section calculation. Construction of a large scale Green’s function is done via expansion of a time dependent evolution operator in Chebyshev polynomials using iterative procedure. Further details can be found in [15].
- Cross section is non-zero only above thresholds, here it is a ground state of an \( N-1 \) nucleus. Near thresholds the kinematics given by the energy dependence of the amplitudes \( A^c(E) \) determines the correct low-energy behavior.
- Cross section curves are generally not symmetric and possess neither Gaussian nor Lorentzian shape. Threshold effects and interferences are essential components.
- For broad resonances identification of resonances (or poles of scattering matrix) with peaks in cross section is ambiguous. An example of this is the controversial case of a broad 1/2\(^-\) resonance in \( ^7\text{He} \). [16, 17, 18, 19]
- Exact symmetries from bound to continuum are important. For example the 5/2\(^-\) state in \( ^7\text{He} \) is not seeing in the cross section since its relatively high spin prevents its decay to the ground state of \(^6\text{He} \). This observation is confirmed experimentally [18].

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