Discrete and continuum spectra in the unified shell model approach

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A new version of the nuclear shell model unifies the consideration of the discrete spectrum, where the results agree with the standard shell model, and continuum. The ingredients of the method are the non-Hermitian effective Hamiltonian, energy-dependent one-body and two-body decay amplitudes, and self-consistent treatment of thresholds. The results for helium and oxygen isotope chains well reproduce the data.

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The standard nuclear shell model (SM) approach erects a wall between the description of intrinsic structure and reactions since it does not account for the continuum spectrum. This problem became acute due to experimental progress towards nuclei far from stability. The proximity of continuum in loosely bound nuclei influences all their properties which makes necessary a common description of the discrete and continuum spectrum. The classical book \(^1\) formulated the unified approach to nuclear reactions based on the SM. However, only recently realistic practical methods \(^2, 3, 4, 5\) were suggested. Below we formulate a version of the shell model in continuous \(^4\) approach \(^5\) of projecting out the states with no restriction by single-nucleon decays. We work the description of reaction cross sections and decay amplitudes, and constructing the effective Hamiltonian \(\mathcal{H}\) that acts in the “internal” \(P\)-space of the many-body SM states \(|\nu\rangle\).

Within the total space \(P + Q\) we solve the Schrödinger equation \(\hat{H}(\alpha) = E(\alpha)\), where the full wave function \(|\alpha\rangle\) is a superposition of internal states \(|\nu\rangle\) and external states \(|c; E\rangle\). The elimination of external states leads to the closed equation for the internal part with the effective Hamiltonian

\[
\mathcal{H}(E) = H + \Delta(E) - \frac{i}{2} W(E),
\]

where the principal value term \(\Delta\) is due to the off-shell processes of virtual excitation into channel space \(Q\),

\[
\langle 1|\Delta(E)|2\rangle = \sum_c \mathcal{P} \int dE' \frac{A_1^*(E')^* A_2^*(E')}{E - E'},
\]

and the explicitly non-Hermitian term

\[
\langle 1|W(E)|2\rangle = 2\pi \sum_{c \text{ (open)}} A_1^*(E)^* A_2^*(E)
\]

represents on-shell decays into the channels open at given energy. The amplitudes \(A_\nu^*(E)\) are the matrix elements \(\langle c; E|H|\nu\rangle\) of the original Hamiltonian between \(Q\) and \(P\) spaces. The two new terms depend on running energy \(E\) so that we deal with a non-Hermitian and energy-dependent Hamiltonian. It is important that the observable quantities, such as the scattering matrix, can be written in terms of the same amplitudes and the Hamiltonian \(\mathcal{H}\). The factorized form \(B\) of \(W\) follows from the unitarity of the \(S\)-matrix.

This formulation is exact. The complex poles of the analytical continuation of \(S(E), E_\nu = E_\nu - (i/2)\Gamma_\nu\), are resonances. Since the decay amplitudes \(A_\nu^*(E)\) must vanish below threshold energy \(E_\nu^{\text{th}}\), their energy behavior complicates the situation making decay non-exponential. On the other hand, this ensures a continuous matching to the conventional SM: below thresholds the same bound states are obtained assuming that \(\Delta(E)\) is included into renormalization of the SM interaction. In this work we use \(m\)-scheme Slater determinants on bound single-particle orbitals in the mean field potential for \(P\)-space basis. The channel states are defined by their asymptotic quantum numbers. A one-particle channel of an \(N\)-body system with quantum numbers \(j\), energy of the particle \(\epsilon_j\), and the residual nucleus in the state \(|\alpha; N - 1\rangle\), so that \(E = E_\alpha + \epsilon_j\), is labelled as \(|c\rangle = b_j^\dagger(\epsilon_j)|\alpha; N - 1\rangle\). The total spin-isospin quantum numbers are restored by the solution if the Hamiltonian respects this symmetry.

We assume that one-body decays are determined by the single-particle part \(\delta\) of the full SM Hamiltonian,

\[
A_\nu^*(E_\alpha + \epsilon_j) = \sum_{\nu} a_{\nu j}^\dagger(\epsilon_j) \langle \alpha; N - 1|\nu, 1; N\rangle,
\]

where \(a_{\nu j}^\dagger(\epsilon)\) describes the single-particle transition from the SM state \(\nu\) into continuum state \(j\) with energy \(\epsilon_j\), mediated by the mean-field interaction \(h\). If the valence space is small, and each single-particle state is uniquely marked by spin-isospin quantum numbers, only one orbital \(\nu\) can couple to a given continuum channel, \(a_{\nu j}^\dagger(\epsilon) = \delta_{\nu j} a_j^\dagger(\epsilon);\) then \(\nu\) can be identified with a continuum index \(j\). The non-Hermitian part of effective Hamiltonian...
tonian becomes \( E = \epsilon_j + E_a \)

\[
\langle 1|W(E)|2 \rangle = 2\pi\delta_{12} \sum_j |a^j(\epsilon_j)|^2 \langle \alpha; N-1|b_j|1; N \rangle^2. \tag{5}
\]

Being in general a many-body operator, in some important cases \( W \) is effectively reduced to a single-particle form. Thus, far from thresholds one can ignore the energy dependence and use the closure to simplify the summation in \( \text{Eq. } 4 \).

\[
\langle 1|W(E)|2 \rangle = 2\pi\delta_{12} \sum_j |a^j| \langle 1; N|b_jb_j|1; N \rangle^2. \tag{6}
\]

As a result, \( W \) becomes a one-body operator that assigns a width \( \gamma_j = 2\pi|a^j|^2 \) to each unstable single-particle state \( j = \nu \) and can be combined with the SM Hamiltonian by introducing complex single-particle energies \( \epsilon_{\nu} = \epsilon_{\nu} - i\gamma_{\nu}/2 \). A similar picture emerges if the residual two-body interaction is weak, and the sum over daughter systems \( \alpha \) in Eq. 4 is dominated by a single term. The single-particle interpretation of the continuum coupling \( W \) is generally valid when the removal of a particle does not lead to a significant restructuring of the mean field. In the lowest order \( \text{Eq. } 4 \), the phenomenon of decay does not change the structure of the internal wave function. The width of the many-body state \( \alpha \) is then given by the expectation value \( \Gamma_\alpha = \langle \alpha|W|\alpha \rangle \); if \( W \) is assumed to be a one-body operator, \( \Gamma_\alpha = \gamma_{\nu}(\epsilon_{\nu})(\alpha|b_\nu^\dagger b_\nu|\alpha) \). This defines a many-body decay width as a product of a single-particle width and the spectroscopic factor \( \langle \alpha|b_\nu^\dagger b_\nu|\alpha \rangle \).

The single-particle decay follows from the one-body scattering problem in an average potential \( V \) that enters the one-body Hamiltonian \( h \); this determines the reduced single-particle amplitudes \( a^\nu(\epsilon) \). Assuming spherical symmetry of \( V(r) \), the single-particle decay amplitude is found as \( a^\nu(\epsilon) = \int_0^\infty F_1(r)V(r)u_\nu(r)dr \), where \( u_\nu \) is the radial function, and (for a neutron interacting pair) \( F_1(r) = (2\mu/\pi k)^{1/2}kr j_1(kr) \). For the near-threshold cases, the continuum admixtures are dominated by the long wavelength states; with \( k \to 0 \) behavior \( F_1(r) \sim (kr)^{l+1} \), then \( a^\nu(\epsilon) \sim e^{(l+1)/2} \).

The two-nucleon decay admixes the two-body continuum in the asymptotic form \( |c \rangle = b_\nu^\dagger(\epsilon)b_j^\dagger(\epsilon')|\alpha; N-2 \rangle \). The channel state is characterized by energies of emitted particles, \( \epsilon \) and \( \epsilon' \). With the one-body interaction used for the single-particle decay, the admixture from the two-particle continuum appears as a second order contribution,

\[
A^\nu_\beta(E) = \sum_\beta a^\nu(\epsilon)a^{\nu'}(\epsilon') \left( \frac{b_j^\dagger(\epsilon)b_j^\dagger(\epsilon')}{E - E_\beta} + (j \leftrightarrow j') \right), \tag{7}
\]

that proceeds through intermediate states \( \beta \) of a nucleus with \( N-1 \) particles. Eq. 4 and corresponding contribution to \( W \), Eq. 3, allow for additional simplifications in the near-threshold region. The overall width behaves as \( \gamma \sim q^{2+\epsilon} \), where \( q \) is the total available kinetic energy.

In contrast to this sequential decay amplitude, a direct two-body transition requires the presence of a two-body interaction in the Hamiltonian. To describe this process, a pair amplitude is introduced,

\[
A^\nu_\beta(E) = \langle \alpha, N-2|p_\nu|1; N \rangle \text{ where operator } p_\nu = \{b_\nu \otimes \bar{b}_\nu^\dagger \} \text{ removes a pair, and only the quantum numbers } L \text{ of the pair are conserved. In the long wavelength limit, the two-body decay amplitude scales with energy in accordance with the phase space volume, identically to the sequential decay. The dominant contribution of orbital momentum } L = 0 \text{ results in } W \sim q^2; \text{ this “pairing” channel is also favored by the short-range nature of residual forces.}

As a first application, we consider the chain of helium isotopes from \(^4\text{He} \) to \(^{10}\text{He} \). The internal \( P \)-space contains two single-particle levels, \( p_{3/2} \) and \( p_{1/2} \). The interaction and single-particle energies are defined in \( \text{Eqs. } 4 \) and \( \text{Table I} \). For the one-body channels, using the Woods-Saxon potential with the parameters adjusted for \(^5\text{He} \), it was determined that, even for several MeV above threshold, the single-particle amplitudes can be described by the parameterization \( \gamma_{3/2}(\epsilon) = 0.608 \epsilon^{3/2} \text{MeV} \) and \( \gamma_{1/2}(\epsilon) = 0.3652 \epsilon^{3/2} \text{MeV} \) for the decay width from \( p_{3/2} \) and \( p_{1/2} \) states, respectively. The sequential two-body decay is computed using Eq. 4 with the near-threshold approximation for the energy dependence of single-particle amplitudes. The direct two-body decay is introduced only for the pair emission with total angular momentum \( L = 0 \). It is assumed that all internal \( L = 0 \) pairs couple to the continuum with the same amplitude \( a^{(L=0)}(\epsilon_1, \epsilon_2) \). The direct two-body amplitude is parameterized as \( a^{(L=0)}(\epsilon_1, \epsilon_2) = (\epsilon_1 + \epsilon_2)/3\sqrt{2\pi} \), where the numerical constant fixes the strength of the residual two-body interaction. This is the only parameter of the model, and it was adjusted to two-body decays of \(^6\text{He} \). Figure II and Table II show the results of the CSM calculation in a good agreement with data.

Several features are worth emphasizing. (i) By design of the model with \( \Delta(E) \) approximated by a constant and included in the adjusted SM Hamiltonian, energies of bound states agree exactly with the results of the standard SM. The ground states of \(^4\text{He} \), \(^6\text{He} \) and \(^8\text{He} \) are nucleon-stable in agreement with experiment. (ii) Energies of resonances deviate from the SM predictions — the continuum is restructuring internal states. For narrow separated resonances the effect is small. However, in systems strongly coupled to continuum, internal phase transitions with formation of broad (super-radiant) and very narrow states can be found, see [II] and references therein. A similar effect can be traced in Table II so that decaying states are “pushed” further into continuum. (iii) A detailed comparison reveals information about structure and dominant decay modes. The decay of the \( 2^+ \) state in \(^6\text{He} \) is a sequential two-body process.
leading to the ground state of $^4$He with no effects of direct $L = 2$ pair emission. This is not the case for the $0^+_2$ state, where one-body and sequential two-body decays reproduce only about half of the observed width. The rest comes from the direct two-body emission of $L = 0$ neutron pair to the ground state of $^4$He favored since the $0^+_2$ state is mainly a coherent excitation of a neutron orbital. The largest deviation from experiment is seen for the $3/2^-$ state in $^7$He (although the data also have a large uncertainty). Possibly, the direct pair decay to $3/2^-$ state in $^4$He (as seen from Table, it is very important) is followed by a fast further breakdown to $^2$He. Sequential three-body decays were not considered in the model. The admixture of the high-lying $3/2^-$ state with a large width is also possible. (iv) The results agree with calculations [2, 3] by a different method but with a similar mean field and schematic residual force.

As second application, Fig. 2 we perform a full calculation (all states and all interaction matrix elements in the sd-SM included) for the chain of oxygen isotopes; the first results were reported earlier [7]. As for He isotopes, self-consistency is established at all stages: decay energies for given parent-daughter pairs are consistent with the reaction processes; decay amplitudes for given states are in agreement with the reaction calculation and SM spectroscopic factors; the effect of decay on intrinsic states is accounted for in the diagonalization of the non-Hermitian energy-dependent Hamiltonian. The model is essentially parameter-free. The standard SM interaction (USD [11] or its slightly modified version for heavier isotopes HBUSD [12]) was used supplemented by a parameterization of one-body continuum coupling found from scattering off the Woods-Saxon potential adjusted for $^{17}$O. Due to scarce experimental data on neutron decays in heavy isotopes, only sequential two-body processes are considered which requires no additional parameters. A comparison with data is shown in the inserts on Fig. 2 for the USD interaction. A number of features similar to those discussed for the helium isotopes can be noticed.

We presented fully realistic CSM calculations and compared results with experiment. The main ingredients of the method are the SM with a good effective interaction in the discrete spectrum, the non-Hermitian effective Hamiltonian for open channels, correct energy dependence of the decay amplitudes, and the self-consistent calculation of thresholds for a chain of isotopes. The high quality SM results for discrete states are reproduced by the CSM exactly. The comparison with experiment indicates similar high quality for resonances in the continuum. A model requires very few parameters, and most of them can be fixed via simplified calculations of scattering processes. The self-consistency between reactions and structure through energy dependence, thresholds, and parent-daughter relations is a part of the method. Consideration of continuum goes beyond single-particle processes. A detailed study of one- and two-body decays and comparison with data provide insight into structure of resonant states and interplay of intrinsic and continuum dynamics.

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**FIG. 1:** Results for He isotopes. For each isotope CSM result is on the left, while experimental value is to the right; experimentally observed states are linked to theorectical counterparts. The decay width is shown on the right in the units of MeV. Energies (or centroids of decaying states) are not shown, but the energy scale is given on the vertical axis.

<table>
<thead>
<tr>
<th>$^4$He</th>
<th>$^6$He</th>
<th>$^8$He</th>
<th>$^{10}$He</th>
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<tr>
<td><strong>CSM</strong></td>
<td><strong>EXP</strong></td>
<td><strong>CSM</strong></td>
<td><strong>EXP</strong></td>
</tr>
<tr>
<td>$E_{1/2^-}$</td>
<td>$E_{3/2^-}$</td>
<td>$E_{5/2^-}$</td>
<td>$E_{7/2^-}$</td>
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<td>6.00 MeV</td>
<td>7.58 MeV</td>
<td>10.1 MeV</td>
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</table>

**TABLE I:** Comparison of the traditional SM and CSM with data for He isotopes. First two columns identify the mass number and spin of the state. Next five columns compare energies: E(SM) traditional SM; E(a) version of CSM with only one-body decays included; E(b) version of CSM with one-body decay and its second order contribution to the two-body process; E(CSM) full CSM including the direct two-body decay mode; E(EX) experimental data, if available. Next five columns compare decay widths from CSM calculations with experimental values; the SM calculation gives only discrete energies. All numbers are given in MeV; energies are measured from the ground state of $^4$He.
FIG. 2: CSM calculations for oxygen isotopes with the HBUSD interaction. States from yellow (long lifetime) to red (short lifetime) are resonance states. The insert on the upper right shows a more detailed picture for the lightest $^{16}$O to $^{19}$O isotopes. Decays from all states that are experimentally measured are shown with arrows. A full comparison between available data and the calculation is given for $^{19}$O. Energies are expressed in units of keV. Comparison of widths with available data is given in the table in lower-left corner. For both inserts the interaction USD was used that works better in this mass region.

<table>
<thead>
<tr>
<th>A</th>
<th>Jπ</th>
<th>Experiment</th>
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<td>E(MeV)</td>
<td>Γ(keV)</td>
<td>E(MeV)</td>
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<tr>
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<td>96</td>
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<tr>
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<td>1+</td>
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</tr>
<tr>
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<td>3/2+</td>
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