A study of nuclei of astrophysical interest in the continuum shell model

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Abstract. We present here the first application of realistic shell model (SM) including coupling between many-particle (quasi-)bound states and the continuum of one-particle scattering states to the spectroscopy of $^8$B and to the calculation of astrophysical factors in the reaction $^7$Be$(p, \gamma)^8$B.

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1. Introduction

The theoretical description of weakly bound exotic nuclei close to the drip-line is one of the most exciting challenges today. What makes this subject both particularly interesting and difficult, is the proximity of the particle continuum implying strong modification of the effective nucleon–nucleon interaction and causing unusual spatial properties of the nucleon density distribution (halo structures, large diffusivity). Many of those nuclei are involved in the chain of thermonuclear reactions and, in the absence of data at relevant energies, the models of stars rely to certain extent on calculated astrophysical factors (see Bahcall (1989)).

In weakly bound exotic systems, the number of excited bound states or narrow resonances is small and, moreover, they couple strongly to the particle continuum. Hence, these systems should be described in the quantum open system formalism which does not artificially separate the subspaces of (quasi-) bound (the $Q$-subspace) and scattering (the $P$-subspace) states. For well bound nuclei close to the $\beta$-stability line, microscopic description of states in the first subspace is given by nuclear SM with model-space dependent effective two-body interactions, whereas the latter subspace is treated in terms of coupled channels equations. In this work, we question the validity of this basic paradigm of nuclear physics, and propose its modification for weakly stable exotic nuclei by taking into account coupling between $Q$ and $P$ subspaces in terms of residual nucleon–nucleon interaction. This coupling modifies the scattering solutions as well as the spectroscopic quantities for interior bound states.

As said before, we are interested in describing low lying bound and quasi-bound states in exotic nuclei. For that reason, we can restrict description of particle continuum to the subset of one nucleon decay channels. Still, in few rare cases of two-nucleon halo nuclei, this limitation may turn out to be restrictive. In any case, further improvement of our model to more complicated channels like, e.g., $\alpha$-channels, can be done as well (Balashov et al. (1964)).

2. The shell model embedded in the continuum (SMEC)

The influence of scattering continuum on the mean-field properties has been addressed before (see Dobaczewski et al. (1996) for review). No such analysis has been done so far for the realistic SM. A possible starting point could be the Continuum Shell Model (CSM) approach (Fano 1961, Mahaux and Weidenmüller (1969), Philpott (1977)), which in the restricted space of configurations generated using the finite-depth potential, has been studied for the giant resonances and the radiative capture reactions probing the microscopic structure of these resonances (Barz et al. (1977,1978), Fladt et al. (1988)). This is insufficient for nuclei close to drip lines, where it is essential to have a most realistic description of bound state subspace. For that reason, the corner-stone of our approach, called the Shell Model Embedded in the Continuum (SMEC), is the realistic SM itself which is used to generate the $A$-particle wavefunctions. This choice
implies that the coupling between SM states and the one-particle scattering continuum must be given by the residual interaction. In our case, we use the residual interaction in the form:

\[ V = -V_0 (a + bP_{12}^\sigma)\delta(r_1 - r_2) , \]

with \( a + b = 1 \) and \( a = 0.73 \).

The key element of both SMEC and CSM is the treatment of single-particle resonances, which on one side may have an important amplitude inside a nucleus and, on other side, they exhibit asymptotic behaviour of scattering wavefunctions (Bartz et al. 1977). The part of resonance for \( r < r_c \), where \( r_c \) is the cut-off radius, is included in \( Q \) subspace, whereas the remaining part is left in the \( P \) subspace. The wavefunctions of both subspaces are then renormalized in order to ensure the orthogonality of wavefunctions in both subspaces.

In the SMEC calculations, we solve identical equations as in the CSM (Bartz et al. (1977)) but due to specificity of exotic nuclei, ingredients of these calculations are modified. For the bound states we solve the SM problem: \( H_{QQ}\Phi_i = E_i\Phi_i \), using the code ANTOINE (Caurier (1989)). \( H_{QQ} \equiv QHQ \) is identified with the realistic SM Hamiltonian and \( \Phi_i \) are the \( A \)-particle (quasi-) bound wavefunctions. The quasi-bound resonances in the continuum are included as well.

For the continuum part, we solve the coupled channel equations:

\[ (E^{(+)} - H_{PP})\xi^{(+)}_E = 0 , \]

where index \( c \) denotes different channels and \( H_{PP} \equiv PHP \). The sign ± characterizes the boundary conditions, i.e., whether we consider incoming ‘−’ or outgoing ‘+’ scattering waves. In our case, we have ingoing wave in the input channel and outgoing waves in all channels. The structure of \( (A - 1) \) - nucleus is given by the SM, whereas one nucleon occupies a scattering state. The channel states are defined by coupling one nucleon in the continuum to a ‘hole state’ of \( (A - 1) \) - nucleus. The SM wavefunction has an incorrect asymptotic behaviour for states in the scattering continuum. On the other hand, the standard approach consisting of adjusting values of the two-body matrix elements to the experimental data and/or modifying the monopole term of the effective interaction (Dufour and Zuker (1996)), makes the definition of average single-particle field and the radial dependence of the single-particle wavefunctions somewhat arbitrary. Therefore, to generate both single-particle resonances and the radial formfactors of occupied orbits entering the coupling matrix elements \( (1) \) between states in the subspaces \( Q \) and \( P \), we use the finite-depth average potential of Saxon-Woods type with spin-orbit part included. The parameters of the average potential are fitted to reproduce experimental single-particle states, whenever their identification is possible. This is the initial choice of potential, because the microscopic coupling of bound and scattering states generates the correction term to the mean-field which modifies the single-particle wavefunctions for each \( J^\pi \) of the quasi-bound state. This correction term must be carefully taken into account otherwise, the solutions including coupling of \( Q \) and \( P \) subspaces could be non-orthogonal.
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Figure 1. SM with Cohen–Kurath interaction and SMEC (labeled by residual interaction strength $V_0$) vs. experimental $T = 1$ states of $^8$B nucleus. The proton threshold energy is adjusted to reproduce position of the ground state. The shaded regions represent the width of resonance states.

The third system of equations are the coupled channel equations:

$$ (E^+ - H_{PP})\omega_i^{(+)} = H_{PQ}\Phi_i \equiv w_i, \quad (3) $$

with the source term $w_i$, which is given by the SM structure of $A$-particle wavefunction for state $\Phi_i$. These equations define functions $\omega_i^{(+)}$ which describe the decay of quasi-bound state $\Phi_i$ in the continuum. The source $w_i$ couples the wavefunction of $A$-nucleon localized states with $(A - 1)$-nucleon localized states plus one nucleon in the continuum. The formfactor of the source term is given by the same average potential as used in the $P$-space (2). The residual coupling (1) is also identical. The complete solution can be expressed by means of three functions: $\Phi_i$, $\xi_E$ and $\omega_i$:

$$ \Psi_E^c = \xi_E^c + \sum_{i,j}(\Phi_i + \omega_i)(E - H_{QQ}^{eff})^{-1} < \Phi_j | H_{QP} | \xi_E^c >, \quad (4) $$

where $H_{QQ}^{eff} = H_{QQ} + H_{QP}G_P^{(+)}H_{QP}$ is the effective SM Hamiltonian including the coupling to the continuum and $G_P^{(+)}$ is the Green function for the motion of single particle in $P$. Matrix $H_{QQ}^{eff}$ is symmetric and complex. It can be diagonalized by the
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orthogonal transformation: \( \Phi_i \rightarrow \tilde{\Phi}_j = \sum_j b_{ji} \Phi_i \) with complex eigenvalues \( \tilde{E}_i - \frac{i}{2}\tilde{\Gamma}_i \).

The eigenvalues of \( H_{QQ}^{\text{eff}} \) at energies \( E = \tilde{E}_i \) determine the energies and widths of resonance states. With this changes, one obtains:

\[
\Psi_E^c = \xi_E^c + \sum_i \tilde{\Omega}_i [E - \tilde{E}_i + (i/2)\tilde{\Gamma}_i]^{-1} < \tilde{\Phi}_i | H | \xi_E^c > ,
\]

for the wavefunction of continuum state modified by the discrete states and:

\[
\tilde{\Omega}_i = \tilde{\Phi}_i + \sum_c \int_{\varepsilon_c}^{\infty} dE' \xi_{E'}^c (E'^+ - E')^{-1} < \xi_{E'}^c | H | \tilde{\Phi}_i > ,
\]

for the wavefunction of discrete state modified by the continuum states.

3. Results

3.1. Spectroscopy of \(^8\text{B}\) nucleus

As an example of SMEC calculations for bound and resonant states, let us consider the proton-rich nucleus \(^8\text{B}\). Fig. 1 compares SM spectrum for \( T = 1 \) states of \(^8\text{B}\) calculated in the \( p\) - shell using the Cohen and Kurath (1965) (CK) interaction, with those obtained in the SMEC for two different strength \( V_0 \) of the residual interaction \([\text{1}]\). In the SMEC calculations, the Saxon-Woods average potential with parameters: \( U_0 = -31.924 \text{ MeV}, U_{so} = 6.86 \text{ MeV}, R_0 = R_{so} = 2.95 \text{ fm} \) and \( a = a_{so} = 0.52 \) was used as a starting guess. The spectrum of \(^8\text{B}\) does not show large sensitivity to the choice of these parameters. This initial average potential is then modified for each \( J^\pi \) state by the coupling to the continuum. This correction make the average potential deeper, it increases slightly the diffusivity and produces a maximum at the center of the potential. It is the corrected potential which is then used to calculate the radial formfactors of coupling matrix elements and single-particle wavefunctions. The coupling to the continuum mixes the unperturbed SM states. For example for \( V_0 = 1200 \text{ MeV}\cdot\text{fm}^3 \) in \([\text{1}]\), the wavefunction for the first \( 1^+_1 \) resonance has an overlap of 0.992, 0.1 + 0.005 \( i \) and 0.07 + 0.003 \( i \) with unperturbed SM states \( 1^+_1, 1^+_2 \) and \( 1^+_3 \), respectively. The calculated width of \( 1^+_1 \) state is 17 keV and 29 keV for \( V_0 = 650 \) and 1200 MeV·fm\(^3\) respectively. The experimental width for this state is 37 ± 5 keV. One should notice that also the energy difference between \( 2^+_1 \) and \( 1^+_1 \) states is improved by inclusion of the coupling to the continuum.

3.2. Radiative capture reaction \(^7\text{Be}(p,\gamma)^8\text{B} \) at low energies

The \( \beta^+ \) decay of \(^8\text{B}\), which is formed by the reaction \(^7\text{Be}(p,\gamma)^8\text{B} \) at the center of mass (c.m.) energy of about 20 keV, is the main source of high energy solar neutrinos. In the absence of data in this region, the input of standard model for the solar neutrino problem (Bahcall and Ulrich (1988)) should be compared with those of various calculations. In the SMEC, the initial wavefunction \( \Psi_i([^7\text{Be} + p],J^+_1) \) is:

\[
\Psi_i(r) = \sum_{l_aJ_a} \alpha^{J_a} l_a J_a \left( \frac{r}{R} \right) \left[ (Y^{l_a} \times \chi^{J_a})^{J_1} \right]_{m_i} \chi^{J_1} \]

\( \text{(7)} \)
and the final wavefunction $\Psi_f([^8\text{B}])_{J_f=2^+}$ is:

$$
\Psi_f(r) = \sum_{b,l} A_{b,sj_b}^{j_b J_f} u_{b,sj_b}^{J_f(r)} \left[ (Y^b \times \chi^s)^{j_b} \times \chi^{t_f}_{m_f} \right]^{(J_f)}.
$$

$I_t$ and $s$ denote the spin of target nucleus and incoming proton, respectively. $A_{b,sj_b}^{j_b J_f}$ is the coefficient of fractional parentage and $u_{b,sj_b}^{J_f}$ is the s.p. wavefunction in the many-particle state $J_f$. With the wavefunctions $\Psi_i(r)$ and $\Psi_f(r)$, we calculate the transition amplitudes:

$$
T^{EC} = C(EC) i^n \hat{J}_f < 1\delta J_f m_f \mid J_i m_i > < l_0 0 \mid l_0 0 >
\times W(j_b I_l \mathcal{L}_j J_f j_a) W(l_b s \mathcal{L}_j a_j_l_a) I_{a_j_l_a}^{\mathcal{L}_j J_f}
$$

for $E1$ and $E2$ and:

$$
T^{M1} = i^n \mu_N \hat{J}_f < 1\delta J_f m_f \mid J_i m_i >
\times \left\{ W(j_b I_l 1 J_i; J_f j_a) \hat{j}_a j_b
\left[ \mu \left( \frac{Z_i}{m_i^2} + \frac{Z_b}{m_b^2} \right) \hat{l}_a l_a W(l_b s 1 j_a; j_b l_a) + (-1)^{j_b-j_a} 2 \mu_s \hat{s} \hat{s} W(s_l 1 j_a; j_b s) \right]
\right\}
\Delta_a j_b
\Delta_l a_j l a j_b
$$

for $M1$ transitions, respectively. In the above formula, $\delta = m_i - m_f$, $\hat{a} = \sqrt{2a+1}$, $\hat{a} = \sqrt{a(a+1)}$ and $I_{a_j l_a}^{\mathcal{L}_j J_f} = \int u_{l_a j_a} \mathcal{L}_j \psi_{l_a j_a}^{J_f} dr$. The radiative capture cross section can then be expressed in terms of those amplitudes as:

$$
\sigma^{E1,M1} = \frac{16\pi}{9} \left( \frac{k_s^5}{k_p^3} \right)^3 \left( \frac{\mu}{\hbar c} \right) \left( \frac{e^2}{\hbar c} \right)^3 \frac{1}{2s+1} \frac{1}{2I_l+1} \sum | T^{E1,M1} |^2
$$

$$
\sigma^{E2} = \frac{4\pi}{75} \left( \frac{k_s^5}{k_p^3} \right) \left( \frac{\mu}{\hbar c} \right) \left( \frac{e^2}{\hbar c} \right)^2 \frac{1}{2s+1} \frac{1}{2I_l+1} \sum | T^{E2} |^2
$$

Figure 2. Multipole contributions to the total capture cross section (left hand side) and the astrophysical $S$-factor (right hand side) of $^7\text{Be}(p,\gamma)^8\text{B}$ as a function of the center of mass energy. The SMEC calculations has been done with the residual interaction strength $V_0 = 650$ MeV fm$^3$. 
Figure 3. Multipole contributions to the total capture cross section (left hand side) and the astrophysical $S$-factor (right hand side) of $^7$Be$(p, \gamma)^8$B as a function of the center of mass energy. The SMEC calculations has been done with the residual interaction strength $V_0 = 1200$ MeV.fm$^3$.

$\mu$ stands for the reduced mass of the system. Fig. 2 shows the calculated multipole contributions to the total capture cross section and the astrophysical $S$-factor as a function of the c.m. energy. The calculation is done for $V_0 = 650$ MeV.fm$^3$. The proton threshold energy is adjusted to agree energies of calculated and experimental $1^+$ state. The photon energy is given by the difference of c.m. energy of $[^7\text{Be}+p]_{J_i=1}^+$ system and the experimental energy of the $2^+_1$ ground state of $^8$B. The value of the $S$-factor at c.m. energy of 20 keV: $S = 22.58$ eV.b, agrees with certain older experiments (Parker (1966), Kavanagh et al (1969)) but disagrees with the most recent one of Hammache et al (1998).

The ratios of SMEC $S$ factors at different c.m. energies are: $S(20)/S(100) = 1.07$ and $S(20)/S(500) = 1.05$. The ratio of $M1$ and $E1$ contribution is: $\sigma^{M1}/\sigma^{E1} = 8.13\cdot10^{-6}$, $4.55\cdot10^{-5}$ and $4.3\cdot10^{-3}$ at 20, 100 and 500 keV, respectively. The resonant part of $M1$ transitions, which yields the contribution of $S^{M1} = 24.72$ eV.b at the $1^+_1$ resonance energy, decreases fast and becomes $S^{M1} = 9.6\cdot10^{-2}$, $9.6\cdot10^{-4}$, $1.8\cdot10^{-4}$ eV.b at c.m. energies 500, 100, 20 keV, respectively. This value is proportional to the square of spectroscopic amplitude of $p$-states, which for the CK interaction is $-0.352$ and 0.567 for $p_{1/2}$ and $p_{3/2}$ respectively. Similar small values of spectroscopic amplitudes are obtained for Kumar (1974) and PTBME et al (1992) interactions (see Brown et al (1996)). At the position of $1^+$ resonance, the predicted by SMEC calculations value of $S$-factor ($S = 47.05$ eV.b) is smaller than seen in some experiments (Kavanagh et al (1969), Vaughn et al (1970), Filippone et al (1983)). Part of this discrepancy could be related to the absence of quenching factor in our calculations.

Fig. 3 shows the same as Fig. 2 but for $V_0 = 1200$ MeV.fm$^3$. Now, the calculated value of the $S$ factor at c.m. energy of 20 keV is $S = 22.70$ eV.b, rather close to the value obtained for $V_0 = 650$ MeV.fm$^3$, and disagrees with the recent experimental value given by Hammache et al (1998). One should stress however, that different
experiments show significant fluctuations in the extrapolated values of $S$. The ratios of $S$ factors at different c.m. energies: $S(20)/S(100) = 1.07$ and $S(20)/S(500) = 0.997$, show much stronger dependence on energy than seen for $V_0 = 650$ MeV·fm$^3$. The resonant part of $M1$ transitions at the $1^+_1$ resonance energy, yields a somewhat smaller value: $S^{M1} = 18.23$ eV·b, than for $V_0 = 650$ MeV·fm$^3$. Finally, at the position of $1^+$ resonance, the predicted by SMEC calculations value of $S$-factor ($S = 41.97$eV·b) is somewhat smaller than seen in the experiments and for $V_0 = 650$ MeV·fm$^3$.

4. Conclusions

In this work we have shown results of first calculations using the SMEC which couples the realistic SM solutions for (quasi-) bound states with the scattering solutions of one-particle continuum. The application to $^7$Be($p,\gamma)^8$B reaction yields satisfactory description of different components of the radiative capture cross section, including the resonant components. In future, more unstable nuclei should be studied in the SMEC approach to systematically address the problem of effective interactions in the extreme conditions of exotic nuclei. At present, we are applying the SMEC to many other reactions of astrophysical interest such as $^{14}$C($n,\gamma)^{15}$C, $^{16}$O($p,\gamma)^{17}$F, $^{18}$O($n,\gamma)^{19}$O.

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