THOx : A few-body coupled-channels code with core excitations

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Abstract

THOx is a self-contained coupled-channels FORTRAN code that solves the three-body scattering problem consisting on a two-body projectile impinging on a target nucleus using the Continuum-Discretized Coupled-Channels (CDCC) formalism [1]. A key feature of this code is the possibility of including collective excitations of the projectile constituents (commonly referred to as "core excitations"). These capabilities are done with appropriate extensions of the CDCC formalism [2, 3]. Two different continuum discretization methods are used: a pseudo-state method (PS) and a binning method. In the former case, the code diagonalises the projectile two-body Hamiltonian in a Transformed Oscillator Basis (THO), obtained applying an appropriate analytical local scale transformation (LST) to the harmonic oscillator wave functions [4, 5]. In the binning method, continuum states are obtained as a linear superposition (i.e. a wave packet) of the scattering states of the two-body projectile [1, 2]. In addition to the single-particle (few-body) excitation of the between the projectile clusters, possible collective excitations of these clusters can be included. This permits, for example, the description of the projectile states in terms of the particle-plus-rotor (PRM) and particle-plus-vibrator models (PVM). To account for the possible excitation and de-excitation of the clusters during the reaction, a deformed potential can be used between the clusters and the target. To solve the scattering problem, the code computes first the coupling potentials between the considered projectile states. These coupling potentials are later used to solve the system of coupled differential equations, using either the Numerov or the R-matrix method. An algorithm of stabilization is also included, which is particularly suitable for situations for which linear independence is partially lost due to numerical

instabilities, as it happens when closed-channels are included. As in other coupled-channels codes [6], `THOx` provides differential cross sections for each included state as a function of the projectile c.m. scattering angle. Three-body observables, i.e., cross sections as a function of the energy and/or angle of the projectile constituents emitted after the breakup are also computed by means of an appropriate transformation of the computed two-body scattering amplitudes [7]. In addition to the scattering calculations, the program can be used to study several properties of the projectile, such as: bound-state eigenvalues and wave functions, scattering state wave functions and phase-shifts and reduced electric transition probabilities $B(E\lambda)$.

Contents

1. Introduction

The development of new techniques to manage radioactive nuclei and the current activity in radioactive beam facilities around the world have allowed in the last years to explore regions of the nuclear chart far off the stability valley [8, 9]. Many experiments have already been performed and even more are programmed in the next few years to approach closer and closer the drip lines for neutrons and protons. Nuclei close to these lines are weakly bound and a proper description of both their structure and their role in collision processes requires necessarily the inclusion of their unbound states. Some of these weakly bound systems (as ^{11}Be, ^{19}C and many others) can be modelled as core + nucleon [10, 11]. In early studies of these systems, no core excitations were considered, but its importance was soon realized [12]. Here a code for studying weakly bound two-body systems including core excitation is presented.

The Hamiltonian of a two-particle weakly bound system (core plus one valence particle) has three parts: the kinetic energy term, the potential interaction between core and particle, and the core Hamiltonian which takes into account the core excitation (details are given in Sect.II). The traditional approach to find eigenvalues and eigenfunctions for the Hamiltonian consists in integrating the corresponding Schrödinger equation with the proper asymptotic boundary conditions. This provides the bound and the scattering states. However, the unbound states form a continuum and are not normalizable which make them not very convenient for some numerical calculations. An alternative to solve the eigenvalue problem is to diagonalize the Hamiltonian in a basis of square-integrable, L^2, functions. This method is usually referred to in the literature as the Pseudostate Method (PS) [13, 14, 15]. In principle, any complete basis can be used, but in practical calculations the diagonalization has to be done in a truncated basis. Thus, the selection of an appropriate basis is important since it will improve the convergence of the calculations. The code `THOx` uses one PS method based on a local scale point transformation (LST) on the harmonic oscillator wave functions, it is called Transformed Harmonic Oscillator (THO) method. The LST can be generated in several ways. In the present work an analytic transformation proposed by Karataglidis et al. is used [16]. This analytical transformation keeps the simplicity of the HO functions, but converts their Gaussian asymptotic behavior into an exponential one, more appropriate to describe bound systems. This LST has several numerical advantages, namely: i) due to the

analytical form of the transformation, it can be easily implemented in a numerical code and there is no numerical problem to generate as many basis functions as required (in other methods wave functions are generated recursively and errors are accumulated), ii) the LST depends on three parameters that govern the radial extension of the THO basis allowing the construction of an optimal basis for each observable of interest, and iii) convergence with this basis seems to be faster than with other alternatives [17, 4].

In order to solve the eigenvalue problem for the two-particle weakly bound system, including core excitation, the code `THOx` constructs the THO basis and diagonalizes the Hamiltonian in it. As a result, eigenvalues and the corresponding eigenvectors are obtained. Negative eigenvalues give the bound states of the system, while the positive ones provide a discrete representation of its continuum. Once the wave functions are available, the reduced electric transition probability from one state to the rest can be calculated provided with the appropriate transition operator. Since the calculated states in the continuum are discrete, the obtained B(Eλ)'s are also discrete. To compare with experimental distributions of B(Eλ) some smoothing is required. The best way of doing this, when it is possible, is to do the folding of the discrete sequence of B(Eλ) values with the actual continuum wave functions. This provides a continuum B(Eλ) distribution. For that purpose, `THOx` allows to generate the actual continuum wave functions by solving the corresponding Schroedinger equation. These functions can be calculated for any positive energy value and allow: on one hand, to calculate the B(Eλ) distribution directly, and on the other hand perform the mentioned folding for the discrete B(Eλ) distribution obtained with the PS method.

The manuscript is structured as follows: Sects. II and III contain a description of the formalism. In Sect. II the Hamiltonian of the composed two-body system is described. In Sect. III the THO basis is constructed and relevant matrix elements, including different types of possible core excitations, are worked out. The code allows to generate the exact scattering states for the proposed Hamiltonian, this is also described in Sect. III. Diagonalization of the Hamiltonian provides eigenvalues and eigenfunctions of the system. With this information the required B(Eλ) values can be evaluated. The input description of the code is presented in Sect. IV while in Sect. V the sequence of sentences required for compilation is given. Finally, in Sect. VI a detailed input-output test example is discussed.

2. Calculation of projectile states [JAL]

2.1. Effective Hamiltonian

Our purpose is to model our nucleus as a core (c) plus valence particle (v) two-body system where the core is not compulsory frozen as an inert spectator. Therefore, we take into account core degrees of freedom into the motion of the valence particle around the core. Our Hamiltonian will then contain a kinematic term depending on the relative coordinate $\vec{r}$ between valence and core, T_r, an intrinsic core part describing the excitations of the core and a potential term for the interaction between valence and core. So far we can express this as:

$$H = \hat{T}_r + V_{vc}(\vec{r}, \xi) + H_{\rm core}(\xi) \tag{1}$$

where $H_{\rm core}(\xi)$ is the intrinsic Hamiltonian of the core, whose eigenstates will be denoted by $\{\phi_{IM_I}\}$. I, and M_I, are the total spin, and its projection on the z-axis, of the state of the core. Additional quantum numbers, required to fully specify the core states, will be specified below.

The interaction between valence and core described by $V_{vc}(\vec{r}, \xi)$ depends upon the relative coordinate $\vec{r}$, but also on the internal degrees of freedom of the core. However, in the weak-coupling limit, it is customary to separate this valence-core interaction into two terms, one describing the motion of the valence particle in some average potential created by the core, and a additional coupling potential containing all the dependence on the core degrees of freedom:

$$V_{vc}(\vec{r}, \xi) = V_{sp}(\vec{r}) + V_{\rm coup}(\vec{r}, \xi) \tag{2}$$

The *single-particle* potential $V_{sp}(\vec{r})$ describes the motion of the valence particle relative to the core, in absence of core excitation. This motion is characterized by the quantum numbers ℓ, angular momentum, s, spin, and j, total spin of the valence particle. The following terms are considered:

$$\begin{aligned} V_{sp}(r) = V_{cou}(r) + V_c^{\ell}(r) + V_{ls}^{v}(r)\vec{\ell}\cdot\vec{s}_v + V_{ls}^{c}(r)\vec{\ell}\cdot\vec{s}_c + V_{ss}(r)\vec{s}_c\cdot\vec{s}_v \\ + V_{ll}(r)\vec{\ell}\cdot\vec{\ell}' \end{aligned} \tag{3}$$

where:

- $V_{cou}(\vec{r})$ is the Coulomb central

- $V_c^\ell(r)$ = ℓ-dependent nuclear central potential
- $V_{ls}^v(r)$ = spin-orbit potential for valence (spin of valence)
- $V_{ls}^c(r)$ = spin-orbit potential for core (spin of the core)
- $V_{ss}(r)$ = spin-spin potential
- $V_{ll}(r) = \ell \cdot \ell'$ potential

The coupling potential $V_{\rm coup}(r,\xi)$ is responsible for transitions between different core states or different valence configurations (preserving the total angular momentum of the system). It will be specified in the following section.

The eigenstates of the Hamiltonian (1) will be a superposition of several valence configurations and core states, i.e.

$$\Psi_{\varepsilon;JM}(\vec{r},\vec{\xi}) = \sum_{\alpha}^{n_\alpha} R_{\varepsilon,\alpha}(r) \left[\mathcal{Y}_{\ell sj}(\hat{r}) \otimes \phi_I(\vec{\xi})\right]_{JM}. \tag{4}$$

where M is the projection of the total angular momentum J. n_α is the number of channel configurations ($\{l,\, j,I\}$) compatible with the total angular momentum and parity J^π. The set of functions

$$\phi_{\alpha,J,M}(\hat{r},\xi_v,\xi_c) \equiv [\mathcal{Y}_{\ell sj}(\hat{r}) \otimes \phi_I(\xi)]_{JM} \tag{5}$$

is the so-called spin-orbit basis.

The radial functions $R_{\varepsilon,\alpha}(r)$ can be obtained using an expansion in a PS basis, such as the THO basis, denoted as:

$$\langle \vec{r}\xi | n(ls)jIJM\rangle \equiv \Phi^\alpha_{n,JM}(\vec{r},\vec{\xi}) = R^{THO}_{n,\alpha}(r) \left[\mathcal{Y}_{\ell sj}(\hat{r}) \otimes \phi_I(\vec{\xi})\right]_{JM}. \tag{6}$$

where n is an index the labels the states of the basis for a given channel.

In this basis, the states of the system will be expressed as

$$\Psi^{(N)}_{i,JM}(\vec{r},\vec{\xi}) = \sum_{n=1}^{N}\sum_{\alpha}^{n_\alpha} c^i_{n,\alpha,J}\Phi^\alpha_{n,JM}(\vec{r},\vec{\xi}), \tag{7}$$

where i is an index that labels the order of the eigenstate. The coefficients $c^i_{n,\alpha,J}$ are obtained by diagonalization of the full Hamiltonian (1) in a truncated basis ($n = 1, \ldots, N$). This requires the evaluation of the matrix elements of the different parts of the Hamiltonian between different functions. For the core Hamiltonian, these matrix elements are simply given by:

$$\langle n(\ell s) j I J || H_{core}(\vec{\xi}) || n'(\ell' s') j' I' J' \rangle = \delta_{I,I'} \delta_{\alpha,\alpha'} E_I \tag{8}$$

because the basis states are, by construction, eigenstates of $H_{core}(\vec{\xi})$.

For the valence-core Hamiltonian, the expression for the matrix elements depend on the assumed model.

3. Projectile matrix elements in the PS basis [JAL]

The coupling potential $V_{\rm coup}(\vec{r}, \xi)$ is written according to the following multipolar expansion:

$$V_{\rm coup}(\vec{r}, \xi) = \sum_{\lambda\mu} V^{\rm coup}_{\lambda\mu}(r, \xi) Y_{\lambda\mu}(\hat{r}). \tag{9}$$

Since the full potential $V_{coup}(\vec{r}, \xi)$ must be an scalar, the coefficients $V^{\rm coup}_{\lambda\mu}$ correspond to a tensor with the same transformation properties as the spherical harmonics $Y_{\lambda\mu}$.

In many interesting cases, the coefficients $V^{\rm coup}_{\lambda,\mu}(r, \xi)$ factorize in a purely radial part $V^{\rm coup}_{\lambda}(r)$ and an internal part, described by a nuclear transition operator, $\mathcal{T}_{\lambda\mu}$

$$V_{coup}(\vec{r}, \xi) = \sum_{\lambda\mu} V^{\rm coup}_{\lambda}(r) \mathcal{T}^*_{\lambda\mu}(\xi) Y_{\lambda\mu}(\hat{r}). \tag{10}$$

The explicit form for the $\mathcal{T}$ will depend on the specific structure model, and will be specified later.

Diagonalization of the full valence-core Hamiltonian requires the evaluation of the matrix elements of this coupling potential between basis states (6), denoted for short as $|c\rangle \equiv |n'(l's')j'I'J'\rangle$. Explicitly [18],

$$\begin{aligned}\langle c || V_{\rm coup}(\vec{r}, \vec{\xi}) || c' \rangle = \delta_{JJ'} (-1)^{j'+I+J} \left\{ \begin{array}{ccc} j & j' & \lambda \\ I' & I & J \end{array} \right\} \hat{I} \langle \gamma I || \mathcal{T}^*_\lambda || \gamma' I' \rangle \\ \times \langle n(\ell s) j || V_\lambda(r) Y_\lambda || n'(\ell' s') j' \rangle \end{aligned} \tag{11}$$

with $\hat{I} = (2I+1)^{1/2}$ and γ denotes any set of additional quantum numbers required to fully specify the core states. In the expression above, we have adopted the definition of Brink and Satchler [19] for reduced matrix elements, namely,

$$\langle JM|T_{kq}|J'M'\rangle = (-1)^{2k}\langle JM|J'M'Kq\rangle\langle J||T_k||J'\rangle \tag{12}$$

The second line in Eq. (11) can be further expanded as:

$$\begin{aligned}\langle n(ls)j||V_\lambda(r)Y_\lambda||n'(l's')j'\rangle &= \hat{j}'\hat{\ell}\hat{\ell}'(-1)^{\lambda+s+j'+2\ell}\sqrt{\frac{2\lambda+1}{4\pi}}\begin{pmatrix}\ell & \lambda & \ell'\\ 0 & 0 & 0\end{pmatrix}\\ &\times \begin{Bmatrix} j & j' & \lambda\\ I' & I & J\end{Bmatrix}\langle n\ell|V_\lambda^{\rm coup}|n'\ell'\rangle\end{aligned} \tag{13}$$

where $\langle n\ell|V_\lambda|n'\ell'\rangle$ are the radial integrals:

$$\langle n\ell|V_\lambda|n'\ell'\rangle = \int R_{n\ell}(r)V_\lambda(r)R_{n'\ell'}(r)r^2dr. \tag{14}$$

We see that the structure of the core is embodied in the matrix elements $\langle\gamma I||\mathcal{T}^*_\lambda||\gamma' I'\rangle$. In the following subsection, we give explicit expressions for the vibrational and rotor models, used in the `THOx` code.

3.1. Axially symmetric particle-rotor model (PRM)

The particle-rotor model (PRM) [20] assumes that the core has a permanent deformation, and hence its radius will not be longer a constant. Instead, the distance from the center to an arbitrary point in the surface is characterized by a function of the angles θ' and ϕ', defined with respect to intrinsic (*body-fixed*) frame,

$$r(\theta',\phi') = R_0[1+\sum_\lambda \beta_\lambda Y_{\lambda 0}(\theta',\phi')] = R_0+\sum_\lambda \delta_\lambda Y_{\lambda 0}(\theta',\phi') \equiv R_0+\Delta(\hat{r}') \tag{15}$$

where R_0 is an average radius of the core and hence the remaining term (denoted $\Delta(\theta',\phi')$) represents the deviation of the radius for a particular point on the surface from this average radius. The quantities $\delta_\lambda = \beta_\lambda R_0$ are the *deformation lengths*. The function $\hat{\Delta}(\hat{r}')$ is sometimes referred to as shift-function.

If one assumes that the valence-core potential is still a function of the distance between the valence particle and the surface of the core, the interaction potential will follow the same functional dependence as $V(r-R_0)$, but

replacing R_0 by $r(\theta', \phi')$. Choosing a reference frame with the z axis along the symmetry axis:

$$V^{\rm rot}(\vec{r}, \theta', \phi') = V(r - r(\theta', \phi')). \tag{16}$$

This expression is expanded in multipoles as:

$$V^{\rm rot}(r, \hat{r}') = \sum_{\lambda} V_{\lambda}^{\rm rot}(r) Y_{\lambda 0}(\hat{r}') \tag{17}$$

with

$$V_{\lambda}^{\rm rot}(r) = 2\pi \int_{-1}^{1} V(r - \hat{\Delta}(\hat{r}')) Y_{\lambda,0}(\theta', 0) d(\cos\theta') \tag{18}$$

For small deformations, one can perform a Taylor series of the potential (16) in powers of Δ:

$$V^{\rm rot}(r, \hat{r}') \approx V^{\rm rot}(r - R_0) - \frac{dV^{\rm coup}}{dr} \sum_{\lambda} \delta_{\lambda} Y_{\lambda 0}(\hat{r}') \tag{19}$$

Inserting this expansion into Eq. (18) gives for a multipole $\lambda > 0$

$$V_{\lambda}^{\rm rot}(r) = -\delta_{\lambda} \frac{dV^{\rm rot}}{dr} \tag{20}$$

The angular variables in these expressions are referred to the reference frame aligned with the symmetry axis, but can be converted to the laboratory frame (characterized by the variables θ, ϕ) by means of the transformation [see eg. Ref. [19], Eq. (2.24)]:

$$Y_{\lambda 0}(\theta', 0) = \sum_{\mu} \mathcal{D}^{\lambda}_{\mu 0}(\alpha, \beta, \gamma) Y_{\lambda \mu}(\theta, \phi)$$

where $\mathcal{D}$ is the so called $r$otation matrix (or D-matrix). Its arguments α, β and γ are the Euler angles describing the transformation from the body-fixed frame to the laboratory frame.

Replacing this expression in (17):

$$V^{\rm rot}(r, \hat{r}') = \sum_{\lambda\mu} V_{\lambda}^{\rm rot}(r) \mathcal{D}^{\lambda}_{\mu 0}(\omega) Y_{\lambda \mu}(\hat{r}) \tag{21}$$

with $\omega = \{\alpha, \beta, \gamma\}$. Comparing this expression with (10) we can make the correspondence:

$$V_\lambda^{\rm coup}(r) \to V_\lambda^{\rm rot}(r) \tag{22}$$

$$\mathcal{T}^*_{\lambda\mu}(\xi) \to \mathcal{D}^\lambda_{\mu 0}(\omega) \tag{23}$$

where we can identify the internal degrees of freedom ξ with the Euler angles $\{\alpha, \beta, \gamma\}$.

In the rotational model, the core states are also defined in the intrinsic frame and can be characterized by the total angular momentum I and its projection on the symmetry axis, K. These states, denoted $|IK\rangle$, ca be transformed to the laboratory frame as [1]

$$|K; IM\rangle = \frac{\hat{I}}{\sqrt{8\pi^2}} \mathcal{D}^I_{MK}(\omega)|IK\rangle \tag{24}$$

Using the properties of the $\mathcal{D}$ matrix, the matrix elements of the transition operator result

$$\langle K; IM|\mathcal{D}^\lambda_{\mu 0}|K; I'M'\rangle = \langle IM\lambda\mu|I'M'\rangle\langle I'K'\lambda 0|IK\rangle \hat{I}'/\hat{I}, \tag{25}$$

so, making use of Eq. (12), the reduced matrix elements entering Eq. (12) are just

$$\langle K; I\|\mathcal{T}^*_\lambda\|K; I'\rangle = \langle K; I\|\mathcal{D}^\lambda\|K; I'\rangle = \langle I'K'\lambda 0|IK\rangle \hat{I}'/\hat{I}. \tag{26}$$

3.2. Particle-vibrator model (PVM):

In the PVM model [18], the core is assumed to be spherical, but it can undergo vibrations around the spherical shape. The surface is parametrized as

$$r = R_0[1 + \sum_{\lambda,\mu} \alpha^\dagger_{\alpha\mu} Y_{\lambda\mu}(\hat{r})] \equiv R_0 + \Delta(\hat{r}) \tag{27}$$

with $\Delta(\hat{r}) \equiv \sum_{\lambda\mu} \alpha^\dagger_{\alpha\mu} Y_{\lambda\mu}(\hat{r})$ and where $\alpha_{\lambda\mu}$ are to be understood as dynamical variables, given in terms of phonon creation ($b^\dagger_{\lambda\mu}$) and annihilation ($b_{\lambda\mu}$)

[1] This expression is valid for a symmetric rotor. For an asymmetric rigid rotor, there is in general a sum in K, [c.f. Ref. [19], discussion following Eq. (2.21)].

operators as:[2]

$$\alpha_{\lambda\mu} = \frac{\beta_\lambda}{\hat{\lambda}}[b_{\lambda\mu} + (-1)^\mu b^\dagger_{\lambda,-\mu}] \tag{28}$$

where β_λ is the so-called *zero-point amplitude*, defined as the root mean square of α in the ground state (no phonons) of the system (denote $|0\rangle$):

$$\beta^2_\lambda = \langle 0| \sum_\mu \alpha_{\lambda\mu}\alpha^\dagger_{\lambda\mu}|0\rangle \tag{29}$$

As in the rotational case, one assumes that the valence-core potential is dependent on the distance of the valence particle to the surface of the core nucleus and hence

$$V^{\rm coup}(r,\xi) \to V^{\rm vib}(r - (R_0 + \Delta(\hat{r})) \tag{30}$$

We can expand this interaction in a Taylor series about the equilibrium position of the surface ($R = R_0$)

$$V^{\rm vib}(r - (R_0 + \Delta(\hat{r})) = V(r - R_0) - R_0\frac{dV^{\rm vib}}{dr}\Delta(\hat{r}) + \ldots \tag{31}$$

Comparing with the general expression (10), we make the correspondence[3]

$$V^{\rm coup}_\lambda(r) = -R_0\beta_\lambda\frac{dV^{\rm vib}}{dr} \tag{32a}$$

$$\mathcal{T}_{\lambda\mu} = \alpha_{\lambda\mu}/\beta_\lambda \tag{32b}$$

The states of the core are expressed as $|N; IM\rangle$, where N is the number of phonons of a given multipolarity[4]. The first term in (31) cannot alter the number of phonons and hence it has only diagonal matrix elements between

[2]Different authors use slightly different definitions of these operators. In any case, for r to be real $\alpha^\dagger_{\alpha\mu}$ must have the same transformation properties as $Y_{\lambda\mu}$, namely, $\alpha^\dagger_{\alpha\mu} = (-1)^\mu\alpha_{\alpha,-\mu}$.

[3]To maintain the parallelism with the rotational model, the parameter β_λ is incorporated in the radial form factor, but it could have been equally kept in the transition operator.

[4]A generic vibrational mode might contain phonons of different multipolarities. However, we will consider only states containing phonons of a given multipolarity.

nuclear states. The second term, being linear in the amplitude, can connect vibrational states differing by one unit in the number of phonons[5]. For example, for the transition between the ground state of the system for an even nucleus ($N = I = M = 0$) to a one-phonon state of angular momentum I and projection M, we have to evaluate the matrix element

$$\langle 1; IM|\mathcal{T}^*_{\lambda\mu}|0; 00\rangle = \beta_\lambda^{-1}\langle 1; IM|\alpha^\dagger_{\lambda\mu}|0; 00\rangle = \beta_\lambda^{-1}\hat{I}^{-1}\delta_{I,\lambda}\delta_{M,\mu}, \tag{33}$$

and hence

$$\langle 1; I\|\mathcal{T}^*_{\lambda\mu}\|0; 0\rangle = \beta_\lambda^{-1}\langle 1; I\|\alpha^\dagger_{\lambda\mu}\|0; 0\rangle = \hat{I}^{-1}\delta_{I,\lambda}\delta_{M,\mu} \tag{34}$$

And, for the inverse transition

$$\langle 0; 0\|\mathcal{T}^*_{\lambda\mu}\|1; I\rangle = \beta_\lambda^{-1}\langle 0; 0\|\alpha^\dagger_{\lambda\mu}\|1; I\rangle = (-1)^I\delta_{I,\lambda}\delta_{M,\mu}. \tag{35}$$

Of course, for the diagonal terms we have

$$\langle 1; 1\|\mathcal{T}^*_{\lambda\mu}\|1; I\rangle = \langle 0; 0\|\mathcal{T}^*_{\lambda\mu}\|0; 0\rangle = 0. \tag{36}$$

`THOx` allows to consider both rotational and vibrational models. Note however that, for the calculation of the coupling potentials, only central and spin-independent parts of the interaction ($V^\ell(r)$ in Eq. (3)) are deformed.

3.3. Basis functions

To describe the relative motion between the valence and core, we use a PS basis. In particular, we use the Transformed Harmonic Oscillator (THO) basis used in our previous works [5, 17]. We start from the usual Harmonic Oscillator basis, whose radial form is written in spherical coordinates as:

$$R^{HO}_{n\ell} = \mathcal{N}_{n,\ell}\exp\left[-\frac{r^2}{2b^2}\right]\mathcal{L}_n^{\ell+1/2}(r^2/b^2) \tag{37}$$

where ℓ is the quantum numbers corresponding to the angular momemtum, $\mathcal{L}_n^{\ell+1/2}$ are the generalized Laguerre polynomials, b is the oscillator length

[5]If one consider higher terms in the amplitude, it is possible to create or annihilate several phonons, connecting more complex states in the core. See [18] for a more complete picture. We restrain ourselves only to one phonon creation here.

and $\mathcal{N}_{n,\ell}$ is the corresponding normalization constant. The THO basis is obtained by applying a local scale transformation $s(r)$ to the HO basis, i.e.,

$$R^{THO}_{n,\ell}(r) = \sqrt{\frac{ds}{dr}} R^{HO}_{n,\ell}[s(r)], \tag{38}$$

The idea of the transformation is to convert the Gaussian asymptotic behavior of the HO functions into an exponential form [21, 22]. Among the many possible choices for $s(r)$, we use the parametric form of Karataglidis *et al.* [16].

$$s(r) = \frac{1}{\sqrt{2}b}\left[\frac{1}{\left(\frac{1}{r}\right)^m + \left(\frac{1}{\gamma\sqrt{r}}\right)^m}\right]^{\frac{1}{m}}, \tag{39}$$

that depends on the parameters m, γ and the oscillator length b. Note that, asymptotically, the function $s(r)$ behaves as $s(r) \sim \frac{\gamma}{b}\sqrt{\frac{r}{2}}$ and hence the functions obtained by applying this LST to the HO basis behave at large distances as $\exp(-\gamma^2 r/2b^2)$. Therefore, the ratio γ/b can be regarded as an effective linear momentum, $k_{\text{eff}} = \gamma^2/2b^2$, which governs the asymptotic behavior of the THO functions. As the ratio γ/b increases, the radial extension of the basis decreases and, consequently, the eigenvalues obtained upon diagonalization of the Hamiltonian in the THO basis tend to concentrate at higher excitation energies. Therefore, γ/b determines the density of eigenstates as a function of the excitation energy. For the parameter m, we recommend the use of the value $m = 4$, which is one of the choices done in Ref. [16].

Note that, by construction, the family of functions $R^{THO}_{n,\ell}(r)$ are orthogonal and constitute a complete set with the following normalization:

$$\int_0^\infty r^2 |R^{THO}_{n,\ell}(r)|^2 dr = 1\,. \tag{40}$$

Moreover, they decay exponentially at large distances, thus ensuring the correct asymptotic behavior for the bound wave functions. In practical calculations a finite set of functions (38) is retained, and the internal Hamiltonian of the composite system is diagonalized in this truncated basis with N states, giving rise to a set of eigenvalues and their associated eigenfunctions, denoted respectively by $\{\varepsilon_p\}$ and $\{\varphi^{(N)}_{p,\ell}(r)\}$ $(p = 1, \ldots, N \times n_\alpha)$. As the basis size is increased, the eigenstates with negative energy will tend to the exact bound states of the system, while those with positive eigenvalues can be regarded as a finite representation of the unbound states.

After diagonalization one obtains $N \times n_\alpha$ eigenstates. These eigenstates are distributed in the energy spectrum with a density of states which depends on the basis parameters, mainly N and γ/b, and to the continuum structure for the selected Hamiltonian, i.e. presence of resonances or different breakup thresholds. Moreover, this density reflects the momentum distribution of the eigenstates which becomes important to obtain continuous energy or momentum distributions of different observables from their discrete representation in the PS basis [14, 23, 17, 4].

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It is also possible to perform a two-step diagonalization with the focus on reducing the final number of basis wavefunction needed for convergence. The idea is to first diagonalize the single-particle Hamiltonian without core excitations:

$$H_{sp} = \hat{T}_r + V_{sp}(\vec{r}). \tag{41}$$

If we diagonalize this Hamiltonian with N THO functions, we will obtain N eigenfunctions $\varphi_{sp}(r)$ for each configuration α:

$$\varphi^k_{sp,\alpha}(r) = \sum_N R^{THO}_N(r). \tag{42}$$

The final eigenfunctions of the total Hamiltonian will be a linear combination of these eigenfunctions. Within the weak-coupling limit, one may expect the final eigenfunction to be quite similar,i.e. to have a large overlap, with the corresponding single-particle leading configurations. The reason is that we can understand the coupling as a small perturbation to these single-particle wavefunctions. Therefore, it would be possible to obtain a good convergence retaining only a reduced number of the low-lying $\varphi_{sp}(r)$ eigenfunctions, n_{sp}. With this smaller number of functions, we then diagonalize the full, more complex, Hamiltonian obtaining the eigenstates:

$$\Psi^{(n_{sp})}_{i,JM}(\vec{r},\vec{\xi}) = \sum_{n_{sp},\alpha} \varphi^{n_{sp}}_{sp,\alpha}(r) \left[\mathcal{Y}_{\ell sj}(\hat{r}) \otimes \phi_I(\vec{\xi})\right]_{JM}. \tag{43}$$

Notice that the final number of eigenfunction will be smaller and will have a smaller number of components. Same convergence can be obtained either diagonalizing the full Hamiltonian at once or with this two-step diagonalization. However, the final wavefunctions are optimized in the sense that the

reduced number of components might help to keep computational demand under control when used within a reaction framework.

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4. Projectile scattering states [AMM]

The radial functions $R_{\varepsilon,\alpha'}(r)$ appearing in the expansion (4) can be also be obtained solving the Schrödinger equation in differential form. This is done by inserting the Eq. (4) into the Schrödinger equation and projecting onto the channel basis given by $|(\ell s)jIJ\rangle$. This gives rise a set of coupled differential equations for the unknowns $R_{\varepsilon,\alpha'}(r)$ [20].

$$\begin{aligned}\left[-\frac{\hbar^2}{2M}\left(\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}\right)+\varepsilon_I-\varepsilon\right] rR_{\varepsilon,\alpha}(r)\\ +\sum_{\alpha'}\langle(\ell ls)jIJM|V_{vc}(\vec{r},\vec{\xi})|(\ell's')j'I'J'M'\rangle rR_{\varepsilon,\alpha'}(r) &= 0. \end{aligned} \quad (44)$$

with the coupling potentials

$$\begin{aligned}\langle(\ell s)jIJ||V_{vc}(\vec{r},\vec{\xi})||(\ell's')j'I'J'\rangle = \delta_{JJ'}(-1)^{(j'+I+J)}\left\{\begin{array}{ccc} j & j' & \lambda \\ I' & I & J\end{array}\right\}\\ \langle(\ell s)j||Y_\lambda||(\ell's')j'\rangle(2I+1)^{1/2}\langle I||V_\lambda(r,\vec{\xi})||I'\rangle. \end{aligned} \quad (45)$$

where, the specific form of the reduced matrix elements $\langle I||V_\lambda(r,\vec{\xi})||I'\rangle$ will depend on the structure model adopted for the core.

These equations need to be solved subject to the appropriate boundary conditions. For open channels, these boundary conditions impose that, asymptotically, the solution should behave as:

$$u_{\alpha'}(k_{\alpha'},r) \xrightarrow{r\to\infty} \frac{1}{2}ie^{2i\sigma_{\ell'}}\left[\delta_{\alpha'\alpha}H^*_\ell(k_\alpha r)-\left(\frac{v_\alpha}{v_{\alpha'}}\right)^{\frac{1}{2}}S^{(J)}_{\alpha',\alpha}H_{l'}(k_{\alpha'}r)\right], \quad (46)$$

where $u_\alpha(k_\alpha,r) = R_\alpha(k_\alpha,r)r$ (using an obvious notation where the continuum ε label has been replaced by a dependence on the corresponding momentum k) and where $S^{(J)}_{\alpha',\alpha}$ are the S-matrix elements for total angular momentum J. For closed channels, the boundary condition must be replaced by:

$$u_{\alpha'}(k_{\alpha'},r) \xrightarrow{r\to\infty} C_\alpha W_{-\eta,\ell+1}(2\eta_\alpha r) \quad (47)$$

where W is the Whittaker function with Sommerfeld parameter η_α.

5. Electric transition probabilities [JAL]

The accuracy of the PS basis to represent the continuum can be studied by comparing the ground-state to continuum transition probability due to a given operator. Here we consider the important case of the electric dissociation of the initial nucleus into the fragments $c + v$. This involves a matrix element between a bound state (typically the ground state) and the continuum states.

The electric transition probability between two bound states $|J_i\rangle$ and $|J_f\rangle$ (assumed here to be unit normalized) is given by the reduced matrix element (according to Brink and Satchler convention [19])

$$\mathcal{B}(E\lambda; i \to f) = \frac{2J_f + 1}{2J_i + 1} \left|\langle J_f||\mathcal{M}(E\lambda)||J_i\rangle\right|^2, \tag{48}$$

where $\mathcal{M}$ is the multipole operator. In a core+valence model, the electric transition operator can be written as a sum of three terms [24]: one for the excitation of the valence particle outside the core, one for the excitation of the core as a whole and one for mixed excitations involving simultaneous excitations of core and valence particle,

$$\begin{aligned} \mathcal{M}(E\lambda\mu) &= \sum_{k=1}^{\lambda-1} \sum_{m=-k}^{k} f_\lambda(k, m, \mu) \\ &\times \mathcal{M}_{sp}(Ekm)\mathcal{M}_{core}(E(\lambda - k)(\mu - m)) \\ &+ \mathcal{M}_{sp}(E\lambda\mu) + \mathcal{M}_{core}(E\lambda\mu), \end{aligned} \tag{49}$$

where $f_\lambda(k, m, \mu)$ is a well-defined function of its indices and the single particle contribution has the usual form,

$$\mathcal{M}_{sp}(E\lambda\mu) = Z_{\text{eff}}^{(\lambda)} e r^\lambda Y_{\lambda\mu}(\hat{r}), \tag{50}$$

with the effective charge:

$$Z_{\text{eff}}^{(\lambda)} = Z_v \left(\frac{m_c}{m_v + m_c}\right)^\lambda + Z_c \left(-\frac{m_v}{m_v + m_c}\right)^\lambda. \tag{51}$$

In the case of a transition to a continuum of states, $|kJ_f\rangle$, the definition (48) is replaced by (see for example [25]):

$$\frac{d\mathcal{B}(E\lambda)}{d\varepsilon} = \frac{2J_f + 1}{2J_i + 1} \frac{\mu_{vc} k}{(2\pi)^3 \hbar^2} \left|\langle kJ_f||\mathcal{M}(E\lambda)||J_i\rangle\right|^2, \tag{52}$$

with $k = \sqrt{2\mu_{vc}\varepsilon}/\hbar$. Note that the extra factor appearing in Eq. (52) with respect to Eq. (48) is consistent with the convention $\langle kJ|k'J\rangle = \delta(k-k')$ and the asymptotic behavior (46).

Using a finite basis, one may calculate only discrete values for the transition probability. According to Eq. (48), the $B(E\lambda)$ between the ground state (with angular momentum J_i) and the n-th PS is given by

$$\mathcal{B}^{(N)}(E\lambda; \text{g.s.} \to n) = \frac{2J_f+1}{2J_i+1} \left| \langle \Psi^{(N)}_{n,J_f} || \mathcal{M}(E\lambda) || \Psi_{\text{g.s.}} \rangle \right|^2 . \tag{53}$$

In order to relate this discrete representation to the continuous distribution (52) one may derive a continuous approximation to (52) by introducing the identity in the truncated PS basis, i.e.

$$I^{(N)}_{JM} = \sum_{n=1}^{N} |\Psi^{(N)}_{n,JM}\rangle\langle\Psi^{(N)}_{n,JM}| . \tag{54}$$

For $N \to \infty$ this expression tends to the *exact* identity operator for the Hilbert space spanned by the eigenfunctions of the considered Hamiltonian. By inserting (54) into the exact expression (52) we obtain the approximate continuous distribution,

$$\begin{aligned} \frac{d\mathcal{B}(E\lambda)}{d\varepsilon} &\simeq \frac{2J_f+1}{2J_i+1} \frac{\mu_{vc} k}{(2\pi)^3 \hbar^2} \\ &\times \left| \sum_{n=1}^{N} \langle kJ_f | \Psi^{(N)}_{n,J_f} \rangle \langle \Psi^{(N)}_{n,J_f} || \mathcal{M}(E\lambda) || \Psi_{\text{g.s.}} \rangle \right|^2 . \end{aligned} \tag{55}$$

This approach provides a *smoothing* procedure to extract continuous distributions as a function of the asymptotic energy ε (or, equivalently, the linear momentum k), from the discrete distributions obtained with the PS basis [26, 17]. This is particularly convenient in situations in which the calculation performed with the scattering states themselves is not possible, such as in the CDCC method.

6. CDCC calculations [AMM]

For a 3-body scattering problem of the form $a(c+v)+T$, the total WF can be expressed in terms of states with definite total angular momentum

$$\Psi^{3b}_{\vec{K}_0}(\xi, \vec{r}, \vec{R}) = \sum_{\beta, JM} C_{\beta, J_T M_T}(\vec{K}_0) \Psi_{\beta, J_T, M_T}(\vec{R}, \vec{r}, \xi) \tag{56}$$

where $\vec{R}$ is the relative coordinate between the projectile center of mass and the target (assumed so far to be structureless). The label $\beta = \{L, J_p, n\}$ denotes the incident channels compatible with the total angular momentum J_T, where $\vec{L}$ (projectile-target orbital angular momentum) and $\vec{J}_p$ both couple to the total spin of the three-body system $\vec{J}_T$. The functions Ψ_{β,J_T,M_T} are expressed in terms of the basis $\{\Phi^{(N)}_{n,J_p}\}$ as:

$$\Psi_{\beta_0,J_T,M_T}(\vec{R},\vec{r},\xi) = \sum_{\beta} \frac{\chi^{J_T}_{\beta,\beta_0}(R)}{R} \left[Y_L(\hat{R}) \otimes \Phi^{(N)}_{n,J_p}(\vec{r},\xi) \right]_{J_T,M_T}, \tag{57}$$

where the expression between brackets is the so-called channel basis.

The radial coefficients, $\chi^{J_T}_{\beta,\beta_0}(R)$, from which the scattering observables are extracted, are calculated by inserting (57) in the Schrödinger equation, giving rise to a system of coupled differential equations.

$$\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dR^2} + \frac{\hbar^2 L(L+1)}{2\mu R^2} + \epsilon_n - E \right) \chi^{J_T}_{\beta,\beta_0}(R) + \sum_{\beta'} V^{J_T}_{\beta,\beta'}(R)\chi^{J_T}_{\beta,\beta_0}(R) = 0 \tag{58}$$

where ϵ_n denotes the energy of the projectile state n. These equations are to be solved under the condition that the radial functions $\chi^{J_T}_{\beta,\beta_0}(R)$ are regular at the origin and behave asymptotically as:

$$\chi^{J_T}_{\beta,\beta_0}(R) \to e^{i\sigma_L} \frac{i}{2} \left[H^{(-)}_L(K_\beta R)\delta_{\beta,\beta_0} - S^{J_T}_{\beta,\beta_0} H^{(+)}_{L'}(K_\beta R) \right] \tag{59}$$

where σ_L is the Coulomb phase, evaluated at the Sommerfeld parameter of the incident channel, and $S^{J_T}_{\beta,\beta_0}$ are the S-matrix elements, from which the scattering observables are to be constructed.

The coefficients $C_{\beta,J_T M_T}$ in Eq. (56) are obtained imposing that, in the absence of projectile-target interactions, it reduces to a plane wave times the projectile internal state (c.f. Eq. (4.70a) of [27]):

$$C_{\beta,J_T M_T}(\vec{K}_0) = \sum_M \frac{4\pi}{K_0} i^L \langle L M J_p M_p | J_T M_T \rangle Y^*_{LM}(\hat{K}_0) \tag{60}$$

6.1. Coupling potentials with core excitations [RDD & AMM]

The main physical ingredients of these coupled equations are the coupling potentials:

$$V^{J_T}_{\beta,\beta'}(R) = \langle \beta; J_T | V_{ct}(\vec{R},\vec{r},\xi) + V_{vt}(\vec{R},\vec{r}) | \beta'; J_T \rangle, \tag{61}$$

where we follow the notation used in Ref. [2],

$$\langle \hat{R}, \vec{r}, \xi | \beta; J_T \rangle = \left[Y_L(\hat{R}) \otimes \Phi^{(N)}_{n,J_p}(\vec{r}, \xi) \right]_{J_T} . \tag{62}$$

The valence particle-target interaction (V_{vt}) is assumed to be central, and will be represented by a phenomenological optical potential describing the valence particle-target elastic scattering at the appropriate energy per nucleon. On the other hand, the core-target interaction is assumed to contain a non-central part, responsible for the dynamic core excitation/deexcitation mechanism. In general, this interaction can be expressed in the multipolar form:

$$V_{ct}(\vec{R}, \vec{r}, \xi) = V_{ct}(\vec{r_c}, \xi) = \sqrt{4\pi} \sum_{Qq} V_{Qq}(r_c, \xi)\ Y_{Qq}(\hat{r}_c), \tag{63}$$

where $\vec{r}_c = \vec{R} - a\vec{r}$, with $a = m_v/(m_v + m_c)$ (m_c and m_v denote the core and valence particle masses, respectively).

The multipole terms $V_{Qq}(r_c, \xi)$ factorize into a radial part and a structure part, i.e.,

$$V_{ct}(\vec{R}, \vec{r}, \xi) = \sqrt{4\pi} \sum_{Qq} \mathcal{V}^Q_{ct}(r_c)\ \mathcal{T}^*_{Qq}(\xi)\ Y_{Qq}(\hat{r}_c). \tag{64}$$

The matrix elements (61) were explicitly evaluated in Ref. [2], giving rise to the expression

$$\begin{aligned} V^{J_T}_{\beta:\beta'}(R) = \hat{L}\hat{L}'\hat{J}_p\hat{J}'_p(-1)^{J_p+J_T} \sum_{\Lambda} (-1)^{\Lambda}\hat{\Lambda}^2 \\ \times \begin{pmatrix} \Lambda & L & L' \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} J_p & J'_p & \Lambda \\ L' & L & J_T \end{Bmatrix} F^{\Lambda}_{J_p n:J'_p n'}(R) \ . \end{aligned} \tag{65}$$

The form factors, $F^{\Lambda}_{J_p n:J'_p n'}(R)$ are given by

$$F^{\Lambda}_{J_p n:J'_p n'}(R) = \sum_{KQ\lambda\alpha,\alpha'} \mathcal{R}^{KQ\lambda}_{\alpha n:\alpha' n'}(R)\ P^{KQ\lambda:\Lambda}_{\alpha:\alpha'} \ , \tag{66}$$

with the radial integral:

$$\mathcal{R}^{KQ\lambda}_{\alpha n:\alpha' n'}(R) = \hat{K} \int u^{J_p *}_{n,\alpha}(r) \mathcal{V}^{QK}_{ct}(r, R) R^{\lambda}(ar)^{Q-\lambda} u^{J'_p}_{n',\alpha'}(r) \mathrm{d}r \ , \tag{67}$$

where

$$\mathcal{V}_{ct}^{QK}(r,R) = \frac{1}{2}\int_{-1}^{+1} \frac{\mathcal{V}_{ct}^{Q}(r_c)}{r_c^Q} P_K(u)\mathrm{d}u\,;\ u = \hat{R}\cdot\hat{r}\ . \tag{68}$$

The coefficients $P_{\alpha:\alpha'}^{KQ\lambda:\Lambda}$ are explicitly written as

$$\begin{aligned} P_{\alpha:\alpha'}^{KQ\lambda:\Lambda} &= (-1)^{j'+\ell+\ell'+s+Q}\hat{Q}^2\hat{K}\hat{j}\hat{j}'\hat{\ell}\hat{\ell}' \\ &\times \begin{pmatrix} K & \lambda & \Lambda \\ 0 & 0 & 0 \end{pmatrix} \sqrt{\frac{(2Q)!}{(2\lambda)![2(Q-\lambda)]!}} \langle I\|\mathcal{T}_Q(\xi)\|I'\rangle \\ &\times \sum_{\Lambda'} \hat{\Lambda}'^2 \begin{pmatrix} K & Q-\lambda & \Lambda' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \Lambda' & \ell & \ell' \\ 0 & 0 & 0 \end{pmatrix} \\ &\times \begin{Bmatrix} \Lambda' & \Lambda & Q \\ \lambda & Q-\lambda & K \end{Bmatrix} \begin{Bmatrix} j & j' & \Lambda' \\ \ell' & \ell & s \end{Bmatrix} \begin{Bmatrix} J_p & J'_p & \Lambda \\ j & j' & \Lambda' \\ I & I' & Q \end{Bmatrix}\ , \end{aligned} \tag{69}$$

which, in addition to geometric coefficients, contain the structure reduced matrix elements $\langle I\|\mathcal{T}_Q(\xi)\|I'\rangle$. Specific models enter into these expressions through the radial form factors $\mathcal{V}_{ct}^{Q}(r_c)$ and the structure reduced matrix elements.

For the Coulomb part of the core-target interaction, we use the usual multipole expansion

$$V_{ct}^{\mathrm{coul}}(\vec{r}_c,\xi) = \sum_{Q,q} \frac{4\pi}{2Q+1}\ \frac{Z_t e}{r_c^{Q+1}}\ \mathcal{M}(EQq)\ Y_{Qq}(\hat{r}_c), \tag{70}$$

where $\mathcal{M}(EQq)$ is the multipole electric operator. Comparing with the general expression (63) we have

$$V_{Qq}(r_c,\xi) \equiv \frac{\sqrt{4\pi}}{2Q+1}\ \frac{Z_t e}{r_c^{Q+1}}\ \mathcal{M}(EQq). \tag{71}$$

For the nuclear part of the core-target interaction, we follow the same approach as for the valence-core interaction, that is, we start with a central interaction, $V_{ct}^{(0)}(r_c)$, that is deformed assuming a quadrupole deformation characterized by a deformation length δ_2.

The resulting potential is expanded in spherical harmonics and transformed to the laboratory frame:

$$V_{ct}^{\rm nuc}(r_c,\theta,\phi) = \sqrt{4\pi}\sum_{Qq} \mathcal{V}_{ct}^{Q}(r_c)\ \mathcal{D}_{q0}^{Q}(\alpha',\beta',\gamma')\ Y_{Qq}(\hat{r}_c) \tag{72}$$

with $\{\alpha',\beta',\gamma'\}$ the corresponding Euler angles and the radial form factors

$$\mathcal{V}_{ct}^{Q}(r_c) = \frac{\hat{Q}}{2}\int_{-1}^{1} V_{ct}^{\rm nuc}\left(r_c - \delta_2 Y_{20}(\theta',0)\right) P_Q(u)\ {\rm d}u, \tag{73}$$

with $u=\cos(\theta')$.

6.2. Couplings potentials with target excitations [MGR & AMM]

6.3. Solving the coupled equations [AMM]

6.4. Stabilization procedure [AMM]

7. Three-body observables [RDD & AMM]

7.1. Scattering wave functions

The calculation of the three-body observables demands the knowledge of the *exact* scattering states in the valence+core system. Assuming a given asymptotic relative wave vector $\boldsymbol{k}_I$, and the spins I of the core and s of the valence particle (with projections μ and σ, respectively), the scattering states $\phi^{(+)}_{\mathbf{k}_I;I\mu;s\sigma}(\mathbf{r},\xi_v,\xi_c)$can be written as a linear combination of the continuum states with good angular momentum J,M:

$$\Psi^{(+)}_{\alpha,J,M}(k_I,\mathbf{r},\xi_v,\xi_c) = \sum_{\alpha'} \frac{f^J_{\alpha:\alpha'}(k_I,r)}{r}\phi_{\alpha',J,M}(\hat{r},\xi_v,\xi_c), \tag{74}$$

where the radial functions $f^J_{\alpha:\alpha'}(k_I,r)$ are the solution of the coupled differential equations,

$$\left[E_{\alpha'} - T_{r\ell'} - V^J_{\alpha':\alpha'}\right] f^J_{\alpha:\alpha'}(k_I,r) = \sum_{\alpha''\neq\alpha'} V^J_{\alpha':\alpha''} f^J_{\alpha:\alpha''}(k_I,r), \tag{75}$$

where $E_{\alpha'} = E_\alpha - \epsilon_{I'} + \epsilon_I$, as a consequence of the energy conservation in the nucleon-core system when the latter is in the state I or I', $T_{r\ell'}$ is the relative kinetic energy operator, and $V^J_{\alpha':\alpha''}$ are the matrix elements of the coupling potentials within the spin-basis $|\alpha' JM\rangle$, defined in Eq. (5):

$$V^J_{\alpha':\alpha''}(r) = \langle \alpha' JM|V_{vc}|\alpha'' JM\rangle \tag{76}$$

These radial functions behave asymptotically as a plane wave in a given incoming channel α and outgoing waves in all channels, i.e.:

$$f^J_{\alpha:\alpha'}(k_I, r) \to e^{i\sigma_\ell} \left[F_\ell(k_I r)\delta_{\ell,\ell'} + T^J_{\alpha,\alpha'} H^{(+)}_{\ell'}(k_I r) \right], \tag{77}$$

where σ_ℓ are the Coulomb phase shifts, $F_\ell(k_I r)$ the regular Coulomb function and $T^J_{\alpha,\alpha'}$ the T-matrix, that is directly related to the S-matrix according to:

$$S^J_{\alpha,\alpha'} = \delta_{\alpha,\alpha'} + 2iT^J_{\alpha,\alpha'}. \tag{78}$$

In terms of these good-angular momentum states, the scattering states result:

$$\begin{aligned}\phi^{(+)}_{\mathbf{k}_I;I\mu;s\sigma}(\mathbf{r}, \xi_v, \xi_c) =& \frac{4\pi}{k_I r} \sum_{\ell,j,J,M} i^\ell Y^*_{\ell m}(\hat{k_I}) \langle \ell m s\sigma | j m_j \rangle \\ & \times \langle j m_j I\mu | JM \rangle \sum_{\alpha'} f^J_{\alpha:\alpha'}(k_I, r)\phi_{\alpha',J,M}(\hat{r}, \xi_v, \xi_c),\end{aligned} \tag{79}$$

where $m_j = M - \mu$, and $m = m_j - \sigma$.

7.2. Breakup amplitudes

We derive the breakup transition amplitude $T^{Is;J_0}_{\mu\sigma;M_0}(\boldsymbol{k}_I, \boldsymbol{K})$ connecting an initial state $|J_0 M_0\rangle$ with that of a three-body system (target+core+valence), whose motion is described in terms of the relative momentum, $\boldsymbol{k}_I$, and a c.m. wave vector, $\boldsymbol{K}$, that differs from the initial momentum, $\boldsymbol{K}_0$, in $|J_0 M_0\rangle$. In order to obtain this relationship, we replace the exact three-body wave function by its XCDCC approximation in the exact (prior form) breakup transition amplitude. That is, we take $\Psi_{J_0,M_0}(\boldsymbol{K}_0) \simeq \Psi^{XCD}_{J_0,M_0}(\boldsymbol{K}_0)$ and therefore we can write:

$$T^{Is;J_0}_{\mu\sigma;M_0}(\boldsymbol{k}_I, \boldsymbol{K}) \simeq \langle \phi^{(-)}_{\boldsymbol{k}_I;I\mu;s\sigma} e^{i\mathbf{K}\cdot\mathbf{R}} | V | \Psi^{XCD}_{J_0,M_0}(\boldsymbol{K}_0) \rangle, \tag{80}$$

with the interaction V between the projectile and the target described by a complex potential expressed as follows:

$$V = V_{ct}(\boldsymbol{r}, \boldsymbol{R}, \xi) + V_{vt}(\boldsymbol{r}, \boldsymbol{R}), \tag{81}$$

where, in addition to the projectile coordinates $\boldsymbol{r}$ and ξ, we have the relative coordinate $\boldsymbol{R}$ between the projectile center of mass and the target.

Furthermore, the core-target interaction (V_{ct}) contains a non-central part, responsible for the dynamic core excitation and de-excitation mechanism, while the valence particle-target interaction (V_{vt}) is assumed to be central. The scattering wave functions $\phi^{(-)}_{\boldsymbol{k}_I;I\mu;s\sigma}$ are just the time reversal of those defined in Eq. (79).

We proceed to relate $T^{Is;J_0}_{\mu\sigma;M_0}$ to the discrete XCDCC two-body inelastic amplitudes $T^{i,J_0,J'}_{M_0,M'}(\theta_i,K_i)$, obtained after solving the coupled equations in the XCDCC method and evaluated on the discrete values of $\boldsymbol{K}$, given by the $\{\boldsymbol{K}_i\}=\{\theta_i,K_i\}$ grid. With this aim, and assuming the validity of the completeness relation in the truncated basis, we get:

$$\begin{aligned} T^{Is;J_0}_{\mu\sigma;M_0}(\boldsymbol{k}_I,\boldsymbol{K}) \simeq & \sum_{i,J',M'} \langle \phi^{(-)}_{\boldsymbol{k}_I;I\mu;s\sigma} | \Psi^{(N)}_{i,J',M'} \rangle \\ & \times \langle \Psi^{(N)}_{i,J',M'} e^{i\mathbf{K}\cdot\mathbf{R}} | V | \Psi^{XCD}_{J_0,M_0}(\boldsymbol{K}_0) \rangle \\ = & \sum_{i,J',M'} \langle \phi^{(-)}_{\boldsymbol{k}_I;I\mu;s\sigma} | \Psi^{(N)}_{i,J',M'} \rangle T^{i,J_0,J'}_{M_0,M'}(\boldsymbol{K}), \end{aligned} \tag{82}$$

where the transition matrix elements $T^{i,J_0,J'}_{M_0,M'}(\boldsymbol{K})$ are to be interpolated from the discrete ones $T^{i,J_0,J'}_{M_0,M'}(\theta_i,K_i)$. The overlaps between the final scattering states and the pseudo-states yield the following transition amplitude:

$$\begin{aligned} T^{Is;J_0}_{\mu\sigma;M_0}(\boldsymbol{k}_I,\boldsymbol{K}) \simeq & \frac{4\pi}{k_I} \sum_{J'} \sum_{\ell,m,j} (-i)^\ell Y_{\ell m}(\hat{k}_I) \langle \ell m s\sigma | j m_j \rangle \\ & \times \langle j m_j I\mu | J'M' \rangle \sum_i \mathcal{G}^{i,J'}_\alpha(k_I) T^{i,J_0,J'}_{M_0,M'}(\boldsymbol{K}), \end{aligned} \tag{83}$$

where

$$\mathcal{G}^{i,J'}_\alpha(k_I) = \sum_{\alpha'} \int f^J_{\alpha:\alpha'}(k_I,r) g^J_{i,\alpha'}(r) dr \tag{84}$$

are the overlaps between the radial parts of the scattering states and pseudo-states wave functions. These overlaps are calculated numerically at the energies given by the relative momentum k_I. In practice, we compute the term involving the summation over i in the r.h.s. of Eq. (83) on a uniform momentum mesh, and interpolate this sum at the required k_I values when combining them with the scattering amplitudes. The above expressions can be used within the standard CDCC method (i.e. without core excitations), in which case the core internal degrees of freedom (ξ) are omitted.

7.3. Two- and Three-body observables

The relative and center of mass motion of the core and the valence particle is described by means of the transition amplitudes in Eq. (83), $T^{Is;J_0}_{\mu\sigma;M_0}(\boldsymbol{k}_I, \boldsymbol{K})$ (with the relative momentum $\boldsymbol{k}_I$ and the c.m. wave vector $\boldsymbol{K}$). From these amplitudes we can derive the two-body observables for a fixed spin of the core, I, the solid angles describing the orientations of $\boldsymbol{k}_I$ (Ω_k) and $\boldsymbol{K}$ (Ω_K), as well as the relative energy between the valence and the core, $E_{\rm rel}$. These observables factorize into the transition matrix elements and a kinematical factor:

$$\frac{d^3\sigma^{(I)}}{d\Omega_k d\Omega_K dE_{\rm rel}} = \frac{\mu_{cv} k_I}{(2\pi)^5\hbar^6}\frac{K}{K_0}\frac{\mu_{pt}^2}{2J+1}\sum_{\mu,\sigma,M_0}|T^{Is;J_0}_{\mu\sigma;M_0}(\boldsymbol{k}_I,\boldsymbol{K})|^2, \tag{85}$$

where μ_{cv} and μ_{pt} are the valence-core and projectile-target reduced masses. The integration over the angular part of $\boldsymbol{k}_I$ gives rise to the following expression for the two-body relative energy-angular cross section distributions:

$$\begin{aligned}\frac{d^2\sigma^{(I)}}{d\Omega_K dE_{\rm rel}} =& \frac{1}{2\pi^3\hbar^6}\frac{K}{K_0}\frac{\mu_{pt}^2\mu_{cv}}{2J+1}\frac{1}{k_I} \\ &\times \sum_{J',M',M_0}\sum_{\ell,j}|\sum_i \mathcal{G}^{i,J'}_\alpha(k_I)T^{i,J_0,J'}_{M_0,M'}(\boldsymbol{K})|^2.\end{aligned} \tag{86}$$

The three-body observables, assuming the energy of the core is measured, are given by [23]:

$$\begin{aligned}\frac{d^3\sigma^{(I)}}{d\Omega_c d\Omega_v dE_c} =& \frac{2\pi\mu_{pt}}{\hbar^2 K_0}\frac{1}{2J+1} \\ &\times \sum_{\mu,\sigma,M_0}|T^{Is;J_0}_{\mu\sigma;M_0}(\boldsymbol{k}_I,\boldsymbol{K})|^2\rho(\Omega_c,\Omega_v,E_c),\end{aligned} \tag{87}$$

where the phase space term $\rho(\Omega_c, \Omega_v, E_c)$, i.e., the number of states per unit core energy interval at solid angles Ω_c and Ω_v, takes the form:

$$\begin{aligned}\rho(\Omega_c,\Omega_v,E_c) =& \frac{m_c m_v \hbar k_c \hbar k_v}{(2\pi\hbar)^6} \\ &\times \left[\frac{m_t}{m_v + m_t + m_v(\boldsymbol{k}_c - \boldsymbol{K}_{tot})\cdot\boldsymbol{k}_v/k_v^2}\right].\end{aligned} \tag{88}$$

Here, the particle masses are given by m_c (core), m_v (valence), and m_t (target) while $\hbar\boldsymbol{k}_c$ and $\hbar\boldsymbol{k}_v$ are the core and valence particle momenta in the

final state. The total momentum of the system corresponds to $\hbar \boldsymbol{K}_{tot}$ and the connection with the momenta in Eq. (83) is made through:

$$\boldsymbol{K} = \boldsymbol{k}_c + \boldsymbol{k}_v - \frac{m_p}{M_{tot}} \boldsymbol{K}_{tot}; \quad \boldsymbol{k}_I = \frac{m_c}{m_p} \boldsymbol{k}_v - \frac{m_v}{m_p} \boldsymbol{k}_c \tag{89}$$

with $m_p = m_c + m_v$ and $M_{tot} = m_c + m_v + m_t$ the total masses of the projectile and the three-body system, respectively.

8. Input description

- **SYSTEM namelist**: Zv, Zc, Av, Ac , sn
  - Zv,Zc= valence and core charges
  - Av,Ac=valence and core masses in atomic units
  - *sn*: intrinsic spin of the valence particle.
- **CORESTATES namelist:** *spin*, *parity*, ex, *kband*.
  Intrinsic spin, parity, excitation energy and rotational band of the core.
  A namelist is read for each core state, until an empty namelist is found
- **OUTPUT namelist:** several variables to control the amount of information written in fort.* files
  - *wfout(:)*: index of eigenstate(s) to be printed
  - *checkorth*: select T or F to check orthogonality between final states
  - *verb:* select 0,1,2 to progresively increase the output of the program
  - *solapout(:)*: index of eigenstate(s) whose momentum/energy distribution we select to be printed
- **NAMELIST grid:** radial grid: ng, rmin,rmax,dr
  - *rmin*, *rmax*, *dr*: mininum, maximum and step radius for uniform grid
  - *ng*: number of quadrature points (for quadrature integration) **not implemented yet!**

- **POTENTIAL namelist:** read as many as possible until an empty namelist is found
  - *ptype*: potential type:
    - ptype=1: Woods-Saxon
    - ptype=2: Pöschl-Teller
    - ptype=3: Gaussian
  - *ap*, *at*: projectile/target masses for radius conversion, ie, $R = r0(ap^{1/3} + at^{1/3})$
  - *vl0*, *r0*, *a0*: depth, radius and diffuseness parameters of central potential. For parity-dependent potentials, define the depth as a vector, for example, Vl0(0:2)=-54 -45 -54
  - *Vso*,*rso*, *aso*: parameters of spin-orbit potential (**Only derivative WS potential is implemented!**)
  - *pcmodel*: specifies the particle-core model used.
    - pcmodel=0: PRM model - pcmodel=1: PVM model
  - *lambda*: multipolarity for this coupling
  - *kband*: projection of core spin in intrinsic axis (only used in the PRM model).
  - *cptype*: coupling potential type: -cptype=0: No coupling
    -cptype=1: Derivative WS or WS with new parametres Vcp0,rcp0,acp
    -cptype=2: Numerical projection on multipoles (Y_{20})
    -cptype=3: Idem as 2 with central potential also recalculated (Y_{00})
  - *Vcp0(:)*, *rcp0*, *acp*: parameters of coupling potential (cptype=1)
  - *delta*: deformation length
- **PAULI namelist:** *n*, *l*, *j*. Quantum numbers for s.p. configuration to be removed by Pauli from the diagonalization making use of the Orthogonality Condition Model (OCM).
- **JPSET namelist:** bastype, mlst, gamma, bosc, nho, nsp,exmin, exmax
  - *bastype*: Basis type use to describe the relative motion between the valence and core, represented by $|n(ls)j\rangle$
    bastype=0 for HO basis
    bastype=1 for THO basis

- *nho*: number of HO functions (for either HO or THO bases)
- *nsp*: number of single-particle eigenvalues to be retained for the diagonalization of full H (if nsp=0, use nsp=nho)
- *bosc*: oscillator parameter
- *gamma,mlst*: γ and m parameters for the analytic LST transformation
- *bas2*: Indicates the program how the diagonalization the full Hamiltonian should be performed:
  - bas2=0: Diagonalizes first the single-particle part, using the THO basis, and then uses the resulting eigenstates to diagonalize the full Hamiltonian. If the variable *nsp* is not zero ($nsp < nho$) then this second diagonalization is done using *nsp* eigenstates.
  - bas2=1: Use THO basis for diagonalization of full H
- *vscale*: scale central part of potential for this JPSET

The code will consider the values ℓ=0, 1, ..., $\ell_{\max}$ compatible with the angular momentum coupling $|(\ell s)jI;J\rangle$

- **SCATWF namelist:** calculates scattering states for the same Hamiltonian by direct integration of the Schrödinger equation. These states are used to calculated momentum distributions of PS and smoothing $B(E\lambda)$ discrete distributions
  - *ifcont*: select T to start the plane waves calculations
  - *emin,emax*: minimum and maximum energy for the scattering states
  - *nk:* number of plane waves to be calculated uniformly spaced in linear momentum between *emin* and *emax*
  - *inc:* for multichannel wavefunctions, *inc* is the index specifying the incoming channel
  - *jset:* Angular momentum/parity set according to the JPSET ordering.
  - *writesol:* If true, write overlap between pseusostates and continuum wavefunctions for the specified JPSET.

    Overlaps are written in fort.52 with the following format:

* - The first two lines are just informative.
* The 3rd line corresponds to emin, emax, nk, energy, nex emin, emax, nk = min. energy, max energy, nb of energies (all three given in scatwf namelist energy=T: the NK energies are evenly spaced in energy (otherwise they are evenly spaced in momentum) nex = number of pseudostates to be printed (can be smaller than nho)
* 4th line: index "n" for eigenvalue and its energy
* Then, it follows the overlap $g(k, n)$ for each energy defined in the [emin, emax] mesh
* From this line onwards, the output is repeated for all pseudostates

Overlaps should be normalized to 1 but note that they are defined in momentum (k) so, if the integration is to be performed in energy, a Jacobian is needed. For printing purposes, I also print the absolute value of the overlaps in fort.520

- **BELAMBDA namelist:** calculates the energy distribution of the electric transition between the continuum and the ground state $B(E\lambda; gs \rightarrow n)$
  - *ifbel*: select T to start the calculation
  - uwfgsfile: file including the wave function of the ground state. Format should be equal to wfout(:) output files: fort.10?
  - *lambda:* multipolarity λ of the electric transition $B(E\lambda)$
  - *rms:* mean squared radii of the core in order to incorporate its Elambda contribution (most of cases E2) to the calculation
  - *BElcore:* same as rms, but explicitely giving $B_c(E\lambda(gs \rightarrow I))$

9. Compilation

To Install the THOX program

- Enter the src subdirectory
- Set the BINDIR variable to the directory where the executable file will be installed

- Uncomment the *include XXX.def* line according to your fortran compiler

To clean old files and libraries type:

```
prompt> make clean
```

To compile the libraries and executables type:

```
prompt> make
```

To copy the executable polpot to the directory specified by the BIN variable type:

```
prompt> make  install
```

10. Test examples

10.1. Calculation of projectile states: ^{11}Be case

As an example, we consider the ^{11}Be nucleus, described as ^{10}Be+n. The ^{10}Be core is treated using the rotor model of Ref. [12] (model Be12-b), which assumes a quadrole deformation parameter β_2=0.67. The n+^{10}Be interaction consists of a Woods-Saxon central part, with a fixed geometry ($R = 2.483$ fm, $a = 0.65$ fm) and a parity-dependent strength ($V_c = -54.24$ MeV for positive parity states and $V_c = -49.67$ MeV for negative ones). The potential contains also a spin-orbit part, whose radial dependence is given by the derivative of the same Woods-Saxon shape, and strength $V_{so} = 8.5$ MeV. Only the ground state (0^+) and the first excited state (2^+, $E_x = 3.368$ MeV) are included in the model space. For the valence-core orbital angular momentum, we consider the values $\ell \leq 2$.

To generate the THO basis we use the LST of Eq. (39) with $m = 4$, $b = 1.6$ fm and $\gamma = 1.84$ fm$^{1/2}$. The value of b was determined in order to minimize the ground state energy of ^{11}Be in a small THO basis.

The input example for this case reads:

```
# 11Be=10Be + n using WS potential

 &SYSTEM Zv=0. Av=1.0087
```

```
         Zc=4. Ac=10.013
         jtot=0.5 parity=1   /

&corestates spin=0.0 parity=+1 ex=0.0 /
&corestates spin=2.0 parity=+1 ex=3.368 /
&corestates /

&valence sn=0.5 lmax=2 /

&output wfout(:)=1 2  3 xcdcc=F verb=2 solapout(:)=0  /

&GRID  rmin=0.0 rmax=60.0 dr=0.05 rlast=60 /

&pauli n=0 /

&BASIS bastype=1 mlst=4 gamma=1.84 bosc=1.6
       nho=20 exmin=-10 exmax=10.0 bas2=0 /

&POTENTIAL ptype=1 ap=1 at=0
          vl0(0:2)=-54.4 -49.672 -54.4
          r0=2.483   a0=0.65
          Vso=8.5    rso=2.483  aso=0.65
          pcmodel=0 lambda=2 kband=0
          cptype=3  Vcp0(0:2)=-54.4 -49.672 -54.4
          rcp0=2.483 acp=0.65 delta=1.664 /
 &potental ptype=0 /

&SCATWF  ifcont=T  emin=0.01 emax=10.01  nk=100 il=1 ilout=1  pcon=0 /

&belambda ifbel=F  /
```


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