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

A. M. Moro[a], R. de Diego[a], M. Gómez-Ramos[a], J. A. Lay[c,a]

[a] *Departamento de FAMN, Universidad de Sevilla, Apartado 1065, E-41080 Seville, Spain*
[b] *Centro de Ciências e Tecnologias Nucleares, Instituto Superior Técnico, Universidade de Lisboa, Estrada Nacional 10 (Km 139,7), P-2695–066 Bobadela LRS, Portugal*
[c] *Dipartimento di Fisica Galileo Galilei and INFN, Via Marzolo 8, I-35131 Padova, Italy*

Abstract

THOxis a self-contained coupled-channels fortran code that solves the a three-body scattering problem consisting on a two-body projectile impinging on a target nucleus using the Continuum-Discretized Coupled-Channels (CDCC) formalism [REF]. A key feature of this code is the possiblity of including collective excitations of the projectile constituents (commonly referred to as "core" excitations") or of the target nucleus. These capabilites are done with apropriate extensions of the CDCC formalism.

The projectile continuum states can be obtained with either a pseudo-state method (PS) or a binning method. In the former case, the coe diagonalises the projectile two-body Hamiltonian in a Transformed Oscillator Basis (THO), obtained applying an appropriate analytic local scale transformation (LST) to the harmonic oscillator wave functions.

Internal excitations of the projectile clusters and of the target are included by deforming the corresponding fragment-potentials, using a rotor or vibrational collective models.

To solve the scattering problem, the code computes first the coupling potentials among the projectile+target states. These coupling potentials are later used to solve the system of coupled differential equations, for which several Numerov and R-matrix solutions are available. A algorigthm of stabilization is also included, which is particularly suitable for situations for which linear independence is partially lost due to numerical instabilities [REF].

As in other CDCC implementations, the code proviced differential cross sections for each included state as a function of the projectile c.m. scattering angle. Three-body observables, i.e., cross sectios as a function of the

projectile-fragments energy or angle can be also computed by an apropriate transformation of the computed transition amplitudes [REF RAUL].

In addition to the scattering calculations, the programme can be used for obtaining energy spectra (bound and a representation of unbound states) and the corresponding wave functions of light exotic nuclei that can be treated as two-body systems. The code can also produce the reduced electric transition probabilities, B(Eλ)'s, between the calculated states and its distribution as a function of energy.

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 [1, 2]. 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 [3, 4]. In early studies of these systems, no core excitations were considered, but its importance was soon realized [5]. 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 Schroedinger 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) [6, 7, 8]. 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 appropiate 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 [9]. 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 [10, 11].

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

In the weak-coupling limit, it is customary to separate the 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 bla,bla

The full Hamiltonian is assumed to be of the form:

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

where $H_{\rm core}(\xi)$ is the intrinsic Hamiltonian of the core, whose eigenstates will be denoted by $\{\phi_{IM_I}\}$. Additional quantum numbers, required to fully specify the core states, will be specified below.

In the models considered here, the valence-core interactions is written as the sum of two terms,

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

The *single-particle* potential $V_{sp}(\vec{r})$ describes the motion of the valence particle relative to the core, in absence of core excitation. 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 $V_{coup}(r,\xi)$ 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 n_α is the number of channel configurations ($\{l,\, j,I\}$) compatible with the total angular momentum and parity J^π.

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

$$\langle \vec{r}\xi | n(ls)jIJM\rangle \equiv \Phi^{\alpha}_{n,JM}(\vec{r},\vec{\xi}) = R^{THO}_{n,\alpha}(r) \left[\mathcal{Y}_{\ell sj}(\hat{r}) \otimes \phi_I(\vec{\xi})\right]_{JM}. \tag{5}$$

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

$$\Psi^{(N)}_{i,JM}(\vec{r},\vec{\xi}) = \sum_{n=1}^{N}\sum_{\alpha}^{n_\alpha} c^{i}_{n,\alpha,J}\Phi^{\alpha}_{n,JM}(\vec{r},\vec{\xi}), \tag{6}$$

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:

$$\langle n(\ell s)jIJ||H_{core}(\vec{\xi})||n'(\ell' s')j'I'J'\rangle = \delta_{I,I'}\delta_{\alpha,\alpha'}E_I \tag{7}$$

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

$$V_{coup}(\vec{r},\xi) = \sum_{\lambda} V^{\rm coup}_{\lambda\mu}(r,\xi)Y_{\lambda\mu}(\hat{r}) \tag{8}$$

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, $\mathcal{T}_{\lambda\mu}$

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

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 (5), denoted for short as $|c\rangle \equiv |n'(l's')j'I'J'\rangle$. Explicitly [12],

$$\begin{aligned}\langle c||V_{vc}(\vec{r},\vec{\xi})||c'\rangle = \delta_{JJ'}(-1)^{j'+I+J}\left\{\begin{array}{ccc} j & j' & \lambda \\ I' & I & J \end{array}\right\}\hat{I}\langle\gamma I||\mathcal{T}^{*}_{\lambda}||\gamma' I'\rangle \\ \times\langle n(\ell s)j||V_{\lambda}(r)Y_{\lambda}||n'(\ell's')j'\rangle\end{aligned} \tag{10}$$

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 [13] for reduced matrix elements, namely,

$$\langle JM|T_{kq}|J'M'\rangle = (-1)^{2k}\langle JM|J'M'Kq\rangle\langle J||T_k||J'\rangle \tag{11}$$

The second line in Eq. (10) can be further expanded as:

$$\begin{aligned}\langle n(ls)j||V_{\lambda}(r)Y_{\lambda}||n'(l's')j'\rangle &= \hat{j'}\hat{\ell}\hat{\ell'}(-1)^{\lambda+s+j'+2\ell}\sqrt{\frac{2\lambda+1}{4\pi}}\left(\begin{array}{ccc}\ell & \lambda & \ell' \\ 0 & 0 & 0\end{array}\right) \\ &\times \left\{\begin{array}{ccc} j & j' & \lambda \\ I' & I & J \end{array}\right\}\langle n\ell|V_{\lambda}|n'\ell'\rangle\end{aligned} \tag{12}$$

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

$$\langle n\ell|V_{\lambda}|n'\ell'\rangle = \int R_{n\ell}(r)V_{\lambda}(r)R_{n'\ell'}(r)r^2dr \tag{13}$$

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) [14] 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 characterized by a function of the angles θ' and ϕ'), defined with respect to intrinsic (*body-fixed* frame),

$$r(\theta',\phi') = R_0[1 + \sum_\lambda \beta_\lambda Y_{\lambda 0}(\theta',\phi')] = R_0 + \sum_\lambda \delta_\lambda Y_{\lambda 0}(\theta',\phi')] \equiv R_0 + \Delta(\hat{r}') \tag{14}$$

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:

$$V^{\rm rot}(\vec{r},\theta',\phi') = V(r - r(\theta',\phi')). \tag{15}$$

This expression is expanded in multipoles as:

$$V^{\rm rot}(r,\hat{r}') = \sum_\lambda V^{\rm rot}_\lambda(r) Y_{\lambda 0}(\hat{r}') \tag{16}$$

with

$$V^{\rm rot}_\lambda(r) = 2\pi \int_{-1}^{1} V(r - \hat{\Delta}(\hat{r}')) Y_{\lambda,0}(\theta',0) d(\cos\theta') \tag{17}$$

For small deformations, one can perform a Taylor series of the potential (15) in powers of Δ:

$$V^{\rm rot}(r,\hat{r}') \approx V^{\rm rot}(r - R_0) - \frac{dV^{\rm coup}}{dr} \sum_\lambda \delta_\lambda Y_{\lambda 0}(\hat{r}') \tag{18}$$

Inserting this expansion into Eq. (17) gives for a multipole $\lambda > 0$

$$V^{\rm rot}_\lambda(r) = -\delta_\lambda \frac{dV^{\rm rot}}{dr} \tag{19}$$

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. [13], 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 (16):

$$V^{\rm rot}(r, \hat{r}') = \sum_{\lambda\mu} V^{\rm rot}_{\lambda}(r) \mathcal{D}^{\lambda}_{\mu 0}(\omega) Y_{\lambda\mu}(\hat{r}) \tag{20}$$

with $\omega = \{\alpha, \beta, \gamma\}$. Comparing this expression with (9) we can make the correspondence:

$$V^{\rm coup}_{\lambda}(r) \to V^{\rm rot}_{\lambda}(r) \tag{21}$$

$$\mathcal{T}^{*}_{\lambda\mu}(\xi) \to \mathcal{D}^{\lambda}_{\mu 0}(\omega) \tag{22}$$

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]

$$|K; IM\rangle = \frac{\hat{I}}{\sqrt{8\pi^2}} \mathcal{D}^{I}_{MK}(\omega) |IK\rangle \tag{23}$$

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

$$\langle K; IM | \mathcal{D}^{\lambda}_{\mu 0} | K; I'M' \rangle = \langle IM\lambda\mu | I'M' \rangle \langle I'K'\lambda 0 | IK \rangle \hat{I}'/\hat{I}, \tag{24}$$

so, making use of Eq. (11), the reduced matrix elements entering Eq. (11) are just

$$\langle K; I \| \mathcal{T}^{*}_{\lambda} \| K; I' \rangle = \langle K; I \| \mathcal{D}^{\lambda} \| K; I' \rangle = \langle I'K'\lambda 0 | IK \rangle \hat{I}'/\hat{I}. \tag{25}$$

[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. [13], discussion following Eq. (2.21)].

3.2. Particle-vibrator model (PVM):

In the PVM model [12], the core is assumed to be spherical, but it can undergo vibrations around the spherical shape. The surface is parametrized as

$$r = R_0[1 + \sum_{\lambda,\mu} \alpha^\dagger_{\alpha\mu} Y_{\lambda\mu}(\hat{r})] \equiv R_0 + \Delta(\hat{r}) \tag{26}$$

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 ($b_{\lambda\mu}$) operators as:[2]

$$\alpha_{\lambda\mu} = \frac{\beta_\lambda}{\hat{\lambda}}[b_{\lambda\mu} + (-1)^\mu b^\dagger_{\lambda,-\mu}] \tag{27}$$

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 $|0\rangle$):

$$\beta^2_\lambda = \langle 0| \sum_\mu \alpha_{\lambda\mu} \alpha^\dagger_{\lambda\mu} |0\rangle \tag{28}$$

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

$$V^{\rm coup}(r, \xi) \to V^{\rm vib}(r - (R_0 + \Delta(\hat{r})) \tag{29}$$

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

$$V^{\rm vib}(r - (R_0 + \Delta(\hat{r})) = V(r - R_0) - R_0 \frac{dV^{\rm vib}}{dr} \Delta(\hat{r}) + \dots \tag{30}$$

Comparing with the general expression (9), we make the correspondence[3]

$$V^{\rm coup}_\lambda(r) = -R_0 \beta_\lambda \frac{dV^{\rm vib}}{dr} \tag{31a}$$

$$\mathcal{T}_{\lambda\mu} = \alpha_{\lambda\mu}/\beta_\lambda \tag{31b}$$

[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 paralelism 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.

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 (30) cannot alter the number of phonons and hence it has only diagonal matrix elements between nuclear states. The second term, being linear in the amplitude, can connect vibrational states differing by one unit in the number of phonons. 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

$$\langle 1; IM|\mathcal{T}^*_{\lambda\mu}|0; 00\rangle = \beta_\lambda^{-1}\langle 1; IM|\alpha^\dagger_{\lambda\mu}|0; 00\rangle = \beta_\lambda^{-1}\hat{I}^{-1}\delta_{I,\lambda}\delta_{M,\mu}, \tag{32}$$

and hence

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

And, for the inverse transition

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

Of course, for the diagonal terms we have

$$\langle 1; 1\|\mathcal{T}^*_{\lambda\mu}\|1; I\rangle = \langle 0; 0\|\mathcal{T}^*_{\lambda\mu}\|0; 0\rangle = 0. \tag{35}$$

THOx includes both the rotational and vibrational models. Note however that, the the calculation of the coupling potentials, the central, spin-independent part of the interaction ($V^\ell(r)$ in Eq. (3) is deformed.

3.3. Generic (model independent) matrix elements

In addition to the rotational and vibrational models, it is also possible to define general matrix elements....

3.4. 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 [10, 15]. We start from the usual Harmonic Oscillator basis, whose radial form is written in spherical coordinates as:

$$R^{HO}_{n\ell} = \mathcal{N}_{n,\ell}\exp\left[-\frac{r^2}{2b^2}\right]\mathcal{L}_n^{\ell+1/2}(r^2/b^2) \tag{36}$$

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

where XXXXX. The THO basis is obtained by applying a local scale transformation $s(r)$ to the HO basis, i.e.,

$$R^{THO}_{n,\ell}(r) = \sqrt{\frac{ds}{dr}} R^{HO}_{n,\ell}[s(r)], \tag{37}$$

The idea of the transformation is to convert the Gaussian asymptotic behavior of the HO functions into an exponential form [16, 17]. Among the many possible choices for $s(r)$, we use the parametric form of Karataglidis *et al.* [9].

$$s(r) = \frac{1}{\sqrt{2}b}\left[\frac{1}{\left(\frac{1}{r}\right)^m + \left(\frac{1}{\gamma\sqrt{r}}\right)^m}\right]^{\frac{1}{m}}, \tag{38}$$

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. [9].

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

$$\int_0^\infty r^2 |R^{THO}_{n,\ell}(r)|^2 dr = 1\,. \tag{39}$$

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 (37) 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 [7, 18, 10, 11].

4. Projectile scattering states [AMM]

The radial functions $R_{\varepsilon,\alpha'}(r)$ appearing the expansion (4) can be also be obtained solving the Schrödinger equation in differential form. This is done by inserting the (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 $R_{\varepsilon,\alpha'}(r)$ [14].

$$\begin{aligned} \left[-\frac{\hbar}{2M}\left(\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}\right)+\varepsilon_I-\varepsilon\right] rR_{\varepsilon,\alpha}(r) \\ +\sum_{\alpha'}\langle(\ell ls)jIJM|V_{vc}(\vec{r},\vec{\xi})|(\ell's')j'I'J'M'\rangle rR_{\varepsilon,\alpha'}(r) &= 0. \end{aligned} \tag{40}$$

with the coupling potentials

$$\begin{aligned} \langle(\ell s)jIJ||V_{vc}(\vec{r},\vec{\xi})||(\ell's')j'I'J'\rangle = \delta_{JJ'}(-1)^{(j'+I+J)}\left\{\begin{array}{ccc} j & j' & \lambda \\ I' & I & J \end{array}\right\} \\ \langle(\ell s)j||Y_\lambda||(\ell's')j'\rangle(2I+1)^{1/2}\langle I||V_\lambda(r,\vec{\xi})||I'\rangle. \end{aligned} \tag{41}$$

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:

$$u_{\alpha'}(k_{\alpha'},r) \xrightarrow{r\to\infty} \frac{1}{2}ie^{2i\sigma_{\ell'}}\left[\delta_{\alpha'\alpha}H^*_\ell(k_\alpha r)-\left(\frac{v_\alpha}{v_{\alpha'}}\right)^{\frac{1}{2}}S^{(J)}_{\alpha',\alpha}H_{l'}(k_{\alpha'}r)\right], \tag{42}$$

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:

$$u_{\alpha'}(k_{\alpha'}, r) \quad \xrightarrow{r\to\infty} \quad C_\alpha W_{-\eta,\ell+1}(2\eta_\alpha r) \tag{43}$$

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 [13])

$$\mathcal{B}(E\lambda; i \to f) = \frac{2J_f + 1}{2J_i + 1} \left|\langle J_f || \mathcal{M}(E\lambda) || J_i \rangle\right|^2, \tag{44}$$

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 [19]: 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,

$$\begin{aligned} \mathcal{M}(E\lambda\mu) &= \sum_{k=1}^{\lambda-1} \sum_{m=-k}^{k} f_\lambda(k, m, \mu) \\ &\times \mathcal{M}_{sp}(Ekm)\mathcal{M}_{core}(E(\lambda - k)(\mu - m)) \\ &+ \mathcal{M}_{sp}(E\lambda\mu) + \mathcal{M}_{core}(E\lambda\mu), \end{aligned} \tag{45}$$

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

$$\mathcal{M}_{sp}(E\lambda\mu) = Z^{(\lambda)}_{\text{eff}} e r^\lambda Y_{\lambda\mu}(\hat{r}), \tag{46}$$

with the effective charge:

$$Z_{\rm eff}^{(\lambda)} = Z_v \left(\frac{m_c}{m_v+m_c}\right)^{\lambda} + Z_c \left(-\frac{m_v}{m_v+m_c}\right)^{\lambda}. \tag{47}$$

In the case of a transition to a continuum of states, $|kJ_f\rangle$, the definition (44) is replaced by (see for example [20]):

$$\frac{d\mathcal{B}(E\lambda)}{d\varepsilon} = \frac{2J_f+1}{2J_i+1}\frac{\mu_{vc}k}{(2\pi)^3\hbar^2}\left|\langle kJ_f||\mathcal{M}(E\lambda)||J_i\rangle\right|^2, \tag{48}$$

with $k=\sqrt{2\mu_{vc}\varepsilon}/\hbar$. Note that the extra factor appearing in Eq. (48) with respect to Eq. (44) is consistent with the convention $\langle kJ|k'J\rangle = \delta(k-k')$ and the asymptotic behavior (42).

Using a finite basis, one may calculate only discrete values for the transition probability. According to Eq. (44), the $B(E\lambda)$ between the ground state (with angular momentum J_i) and the n-th PS is given by

$$\mathcal{B}^{(N)}(E\lambda;\,\text{g.s.}\rightarrow n) = \frac{2J_f+1}{2J_i+1}\left|\langle\Psi_{n,J_f}^{(N)}||\mathcal{M}(E\lambda)||\Psi_{\text{g.s.}}\rangle\right|^2. \tag{49}$$

In order to relate this discrete representation to the continuous distribution (48) one may derive a continuous approximation to (48) by introducing the identity in the truncated PS basis, i.e.

$$I_{JM}^{(N)} = \sum_{n=1}^{N} |\Psi_{n,JM}^{(N)}\rangle\langle\Psi_{n,JM}^{(N)}|. \tag{50}$$

For $N\rightarrow\infty$ this expression tends to the *exact* identity operator for the Hilbert space spanned by the eigenfunctions of the considered Hamiltonian. By inserting (50) into the exact expression (48) we obtain the approximate continuous distribution,

$$\begin{aligned}\frac{d\mathcal{B}(E\lambda)}{d\varepsilon} &\simeq \frac{2J_f+1}{2J_i+1}\frac{\mu_{vc}k}{(2\pi)^3\hbar^2} \\ &\times \left|\sum_{n=1}^{N}\langle kJ_f|\Psi_{n,J_f}^{(N)}\rangle\langle\Psi_{n,J_f}^{(N)}||\mathcal{M}(E\lambda)||\Psi_{\text{g.s.}}\rangle\right|^2.\end{aligned} \tag{51}$$

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 [21, 10]. This is particularly convenient in situations in which the calculation 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 $a(c+v)+T$, whe total WF can be expressed in terms of states with definite total angular momentum

$$\Psi^{3b}_{\vec{K}_0}(\xi,\vec{r},\vec{R}) = \sum_{\beta,JM} C_{\beta,J_T M_T}(\vec{K}_0)\Psi_{\beta,J_T,M_T}(\vec{R},\vec{r},\xi) \tag{52}$$

where $\vec{R}$ is the relative coordinate between the projectile center of mass and the target (assumed so far to be structureless). The label $\beta = L, J_p, n_0$ 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:

$$\Psi_{\beta,J_T,M_T}(\vec{R},\vec{r},\xi) = \sum_{\beta'} \frac{\chi^{J_T}_{\beta,\beta'}(R)}{R}\left[Y_{L'}(\hat{R})\otimes\Phi^{(N)}_{n,J_p}(\vec{r},\xi)\right]_{J_T,M_T}, \tag{53}$$

where the expression between brackets is the so-called channel basis. The different quantum numbers are labeled by $\beta' = \{L', J_p, n\}$, where the spin of the target is ignored by now.

The radial coefficients, $\chi^{J_T}_{\beta,\beta'}(R)$, from which the scattering observables are extracted, are calculated by inserting (53) in the Schrödinger equation, giving rise to a system of coupled differential equations.

$$\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dR^2} + \frac{\hbar^2 L(L+1)}{2\mu R^2} + \epsilon_n - E\right)\chi^J_\beta(R) + \sum_{\beta'} V^J_{\beta,\beta'}(R)\chi^J_{\beta'}(R) = 0 \tag{54}$$

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

$$\chi^{J_T}_{\beta,\beta'}(R) \to e^{i\sigma_L}\frac{i}{2}\left[H^{(-)}_L(K_\beta R)\delta_{\beta,\beta'} - S^J_{\beta'\beta}H^{(+)}_{L'}(K_{\beta'}R)\right] \tag{55}$$

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

The coefficients C_{β,J_TM_T} in Eq. (52) are obtained imposing that, in absence of projectile-target interactions, it reduces to a plane wave times the projectile internal state (c.f. Eq. (4.70a) of [22]):

$$C_{\beta,J_TM_T}(\vec{K}_0) = \sum_M \frac{4\pi}{K_0} i^L \langle LMJ_pM_p|J_TM_T\rangle Y^*_{LM}(\hat{K}_0) \tag{56}$$

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

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

$$V^{J_T}_{\beta,\beta'}(R) = \langle \beta; J_T|V_{ct}(\vec{R},\vec{r},\xi) + V_{vt}(\vec{R},\vec{r})|\beta'; J_T\rangle, \tag{57}$$

where we follow the notation used in Ref. [23],

$$\langle \hat{R},\vec{r},\xi|\beta; J_T\rangle = \left[Y_L(\hat{R}) \otimes \Phi^{(N)}_{n,J_p}(\vec{r},\xi)\right]_{J_T}. \tag{58}$$

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]

8. Input description

- **SYSTEM namelist**: *Zv*, *Zc*, *Av*, *Ac*, *Jtot*, *parity*
  - *Zv*,*Zc*= valence and core charges
  - *Av*,*Ac*=valence and core masses in atomic units
  - *Jtot*, *parity*=total core+valence angular momentum and parity
- **CORESTATES namelist:** *spin*, *parity*, *ex*.
  Intrinsic spin, parity and excitation energy of the core. A namelist is read for each core state, until an empty namelist is found
- **NAMELIST valence:** sn, lmax

- *sn*: intrinsic spin of the valence particle.
- *lmax*: maximum valence-core relative orbital angular momentum.

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

- **NAMELIST output:** 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 pauli:** *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).
- **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!**
- **NAMELIST basis:** 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

- **NAMELIST potential:** read as many as possible until an empty namelist is found
  - *ptype*: potential type:
    - ptype=1: Woods-Saxon
    - ptype=2: Potch-Teller
    - ptype=3: Gaussian
  - *ap*, *at*: projectile/target masses for radius conversion, ie, $R = r0ap^{1/3} + at^{1/3}$
  - *vl0*, *r0*, *a0*: depth, radius and diffuseness parameters of central potential. For parity-dependent potentials, define the depth as a vector, por 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

- **NAMELIST scatwf:** calculates scattering states for the same Hamiltonian by direct integration of the Schrödinger quation. 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*
  - *il:* number of incoming channels for the plane waves. **Channels up to il will be calculated. For il<0, only the -ilth channel is calculated**
  - *ilout,eout:* incoming channel and energy for a plane wave to be printed. Energy is as closed to eout as nk,emin,emax allows

- **NAMELIST belambda:** 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. [5] (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. (38) 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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