A versatile R-matrix module including alternative parametrizations

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Abstract. The evaluation of nuclear reaction data within the resolved resonance regime relies on phenomenological R-matrix analyses. In absence of quantitatively reliable microscopic models phenomenological R-matrix manages to reproduce experiment data at high accuracy especially in the resolved resonance regime with a limited number of parameters while unitarity constraints and sum rules are automatically met. However, due to non-trivial mapping between fitting parameters and observables as well as interference effects, standard R-matrix parameters only loosely correlate with observed resonance structures in cross sections making the fitting process challenging. Elegant alternative parametrizations have been introduced by Brune [1] and recently by Park [2] to enforce the agreement between R-matrix parameters and observed resonance positions, thus simplifying the fitting process. In this contribution the alternative parametrizations are compared as well as the successful implementation of Park's parametrization into the R-matrix module of GECCCOS [3] is demonstrated on first examples.

1 Introduction

Reactions in nuclear systems exhibit resonant structure at low incident energies reflecting the discrete levels at these energies. In the absence of quantitatively reliable microscopic models properly describing this complex n-body regime, one has to rely on phenomenological R-matrix analyses of experimental data. Albeit not microscopically based R-matrix theory satisfies all conservation rules and yields consistent reaction data. Conceptionally R-matrix analyses are not limited in energy, but face a practical limit because of the growing number of open channels with increasing energy. In general the nuclear statistical model is well suited for higher energies. However, its applicability for light nuclear systems is questionable and frequently evaluations of light nuclear systems are limited in energy. Despite of the excellent descriptions, the phenomenological R-matrix lacks of predictive power regarding resonances.

The coupled-channels code GECCCOS has been set up at TU-Wien to test and develop new or improve existing methods for reaction calculations. Among others, a versatile R-matrix module is included which provides various options. The calculable R-matrix using the Lagrange-Mesh technique [4] is implemented as well as the phenomenological R-matrix with standard choices for matching radii and boundary parameters. A Hybrid R-matrix approach is supported to combine calculable and phenomenological R-matrix. In addition a reduced R-matrix approach is implemented in order to account for channels that cannot be treated within the standard R-matrix formalism, e.g. breakup reactions. At present this R-matrix module is best suited for analyses of light nuclear systems, but applications to heavier systems are not excluded.

Phenomenological R-matrix theory has proven to be a powerful tool to describe resonant cross sections as found in nuclear systems at low energies. The number of fitting parameters is limited and physical constraints as unitarity and sum rules are automatically satisfied. Due to the non-trivial relationship between R-matrix parameters and observables the former often do not coincide with the observed resonances. In addition resonances may interfere with each other making the fitting process challenging and time consuming.

To address this issue Brune introduced an alternative parametrization [1]. It forces the positions of the R-matrix poles to coincide with observed resonances, thus drastically simplifying the fitting procedure. In addition transformations between the parameters of the alternative and standard R-matrix parameters are provided.

Recently another R-matrix formalism was introduced by Park [2]. Inspired by the alternative parametrization of Brune, coincidence between R-matrix poles and observed resonances is assumed.

In this contribution the three different parametrizations are briefly revisited and compared. First test calculations are demonstrated using an implementation of Park's parametrization in the R-matrix module of GECCCOS [3].

2 R-matrix formalism

The theory was first formulated by Wigner and Eisenbud [5] and has been revisited by many authors, e.g. [4, 6]. The basic assumption is the division of the configuration space in two parts, an interior and an exterior region. In the exterior region only the Coulomb interaction affects

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the collision partners while the nuclear interaction is assumed negligible. The exterior wave function in channel c with incident channel c_0 takes the form

$$u^{\text{ext}}_{(c_0)c}(r) = \begin{cases} C_c \left[I_c(k_c r)\delta_{cc_0} - S_{cc_0} O_c(k_c r) \right] & c \text{ (open)} \\ A_{cc_0} W_{-\eta, l+\frac{1}{2}}(2\kappa_c r) & c \text{ (closed)}, \end{cases} \tag{1}$$

where k_c in Eq. (1) represents the wave number in channel c, and I_c and O_c are asymptotic incoming and outgoing Coulomb functions for open channels, respectively. For closed channels the wave function in the exterior region is a Whittaker function $W_{-\eta,l+\frac{1}{2}}$ with $\kappa_c = |ik_c|$. The coefficients C_c and A_{cc_0} are normalization constants.

The wave function in the interior region reflects all microscopic many-body interactions of the compound nuclear system and is usually not known. The relative motion component of the wave function is assumed to be given by a superposition of basis functions $\phi_j(r)$ [5],

$$u^{\text{int}}_c(r) = \sum_{j=1}^{N} c_{cj} \phi_j(r). \tag{2}$$

The coefficients c_{cj} define the internal wave function $u^{\text{int}}_c(r)$ for which the logarithmic derivative coincides with that of $u^{\text{ext}}_{(c)\,c_0}$ at the interface of the two regions, i.e. the matching radius $r = a$. Finally the R-matrix can be introduced as

$$u^{\text{int}}_c(a) = \sum_{c'} \sqrt{\frac{\mu_c}{\mu_{c'}}} R_{cc'}(E) \left[a u'_{c'}(a) - B_c u_{c'}(a) \right]. \tag{3}$$

The quantity B_c in Eq. (3) known as the boundary parameter is an arbitrary constant which does not affect the observables [4] and μ_c and $\mu_{c'}$ are the reduced masses of channel c and c', respectively. A suitable choice of B_c can be of advantage in the R-matrix analysis. Common choices include e.g. $B_c = 0$ and $B_c = -\ell$ (with ℓ being the angular momentum quantum number in channel c).

Finally, the collision matrix $\mathbf{U}$ (frequently known as S-matrix) can be directly obtained from the R-matrix by

$$\mathbf{U} = \mathbf{Z}_O^{-1} \mathbf{Z}_I \tag{4}$$

with

$$\begin{aligned} Z_{O,cc'} &= (k_{c'}a)^{-1/2} \left[O_c(k_c a)\delta_{cc'} - k_{c'} a R_{cc'} O'_{c'}(k_{c'}a) \right], \\ Z_{I,cc'} &= (k_{c'}a)^{-1/2} \left[I_c(k_c a)\delta_{cc'} - k_{c'} a R_{cc'} I'_{c'}(k_{c'}a) \right]. \end{aligned} \tag{5}$$

Alternatively, Eq. (4) may also be written as

$$\mathbf{U} = 2i\boldsymbol{\rho}^{\frac{1}{2}} \boldsymbol{O}^{-1} \left[\mathbf{1} - \boldsymbol{R}(\boldsymbol{L} - \boldsymbol{B}) \right]^{-1} \mathbf{R} \boldsymbol{\rho}^{\frac{1}{2}} \boldsymbol{O}^{-1} + \boldsymbol{I}\boldsymbol{O}^{-1}, \tag{6}$$

where $\boldsymbol{O}$, $\boldsymbol{I}$, $\boldsymbol{L}$, $\boldsymbol{B}$ and $\boldsymbol{\rho}$ are diagonal matrices with elements O_c, I_c, L_c, B_c and $\rho_c = k_c a_c$, respectively.

The symbol L_c describes the logarithmic derivative of the outgoing Coulomb functions in channel c at the matching radius a_c

$$L_c = a_c \left(\frac{1}{O_c} \cdot \frac{\partial O_c}{\partial r_c} \right)_{r_c = a_c} = S_c + i\, P_c, \tag{7}$$

where S_c and P_c are known as the shift and penetration factor, respectively.

Using the collision matrix $\mathbf{U}$ from Eq. (4), the scattering amplitude together with all observables can be derived (see e.g. [4]).

The standard R-matrix can be parametrized in a simple way as a sum of pole terms (see e.g. [4–6])

$$R_{cc'}(E) = \sum_{\lambda} \frac{\gamma_{\lambda c} \gamma_{\lambda c'}}{E_\lambda - E}, \tag{8}$$

where E_λ represent the real-valued pole energies and $\gamma_{\lambda c}$ the so-called reduced width amplitudes.

For calculations of the calculable R-matrix within potential theory the number of pole terms is equal to the number of channels times the number of basis functions.

In phenomenological R-matrix analysis the reduced width amplitudes $\gamma_{\lambda c}$ as well as pole energies E_n are fitting parameters adjusted to reproduce observables from experiments. This approach gives an excellent description of experimental data especially for light nuclear systems at low energies. However, due to the non-linear relation between R-matrix parameters (E_λ and $\gamma_{\lambda c}$) and the collision matrix $\mathbf{U}$ the observed resonance positions and widths do not necessarily coincide with the R-matrix parameters. Furthermore interference effects between pole terms in the same partial wave can make the fitting procedure challenging and time consuming. Hence the fitting process becomes more difficult with rising energy and an increasing number of resonances in the cross sections. In order to simplify the fitting procedure of R-matrix analyses the development of alternative parametrizations is of interest.

2.1 Brune Parametrization

Without derivation, Brune's alternative R-matrix parametrization [1] is briefly revisited in this section. It is well-known [7, 8] that choosing the boundary parameter $B_c = S_c(E_\lambda)$ the R-matrix pole position E_λ and the observed resonance energy in the cross section become identical, but only for the pole at $E = E_\lambda$. As mentioned in Sec. 2, the choice of a constant boundary parameter B_c is arbitrary. When changing the boundary parameter, the R-matrix parameters E_λ and $\gamma_{\lambda c}$ can be easily transformed as described in [9], keeping all observables unchanged.

Generalizing the parameter transformation and formulating a non-linear eigenvalue equation, an alternative R-matrix $\tilde{\boldsymbol{R}}$ could be formulated [1] with

$$\tilde{\boldsymbol{R}} = \tilde{\boldsymbol{\gamma}}^T \boldsymbol{Q} \tilde{\boldsymbol{\gamma}}, \tag{9}$$

where $\tilde{\boldsymbol{\gamma}}$ are the alternative reduced width amplitudes $\gamma_{c\lambda}$ in matrix form and $\boldsymbol{Q}$ defined by its inverse

$$\begin{aligned} \left(\boldsymbol{Q}^{-1} \right)_{\lambda\lambda'} = &\left(\tilde{E}_\lambda - E \right) \delta_{c'c} - \sum_c \tilde{\gamma}_{\lambda c} \tilde{\gamma}_{\lambda' c} S_c \\ &+ \sum_c \begin{cases} \tilde{\gamma}^2_{\lambda c} S_{\lambda c} & \lambda = \lambda' \\ \tilde{\gamma}_{\lambda c} \tilde{\gamma}_{\lambda' c} \frac{S_{\lambda c}(E - \tilde{E}_\lambda) - S_{\lambda' c}(E - \tilde{E}'_\lambda)}{\tilde{E}_\lambda - \tilde{E}'_\lambda} & \lambda \neq \lambda', \end{cases} \end{aligned} \tag{10}$$

where $\tilde{E}_\lambda$ are the alternative formal pole positions.

The scattering matrix can be formulated in terms of the new parameters

$$\mathbf{U} = 2i\boldsymbol{\rho}^{\frac{1}{2}}\boldsymbol{O}^{-1}\left[\mathbf{1} - i\tilde{\boldsymbol{R}}\boldsymbol{P}\right]^{-1}\tilde{\mathbf{R}}\,\boldsymbol{\rho}^{\frac{1}{2}}\boldsymbol{O}^{-1} + \boldsymbol{I}\boldsymbol{O}^{-1}. \tag{11}$$

The alternative R-matrix has the striking property that the formal pole positions $\tilde{E}_\lambda$ coincide with the observed resonance positions in the cross sections. There also exist transformations for the reduced widths and pole positions from Brune parametrization to conventional R-matrix and back.

2.2 Park Parametrization

Another alternative R-matrix parametrization, inspired by Brune's work, was proposed by Park [2]. Dropping orthonormality constraints for the basis functions $\phi_j(r)$ in Eq. (2) and allowing a level dependent boundary parameter ($B_c \rightarrow B_{\lambda c}$) leads to new degrees of freedom.

The non-diagonal part of the non-orthogonality term $J_{\lambda\lambda'}$ of the basis functions can be written as

$$J_{\lambda\lambda'} = -\frac{1}{\bar{E}_\lambda - \bar{E}_{\lambda'}}\sum_c \bar{\gamma}_{\lambda c}\left(B_{\lambda c} - B_{\lambda' c}\right)\bar{\gamma}_{\lambda' c} \quad \text{for } \lambda \neq \lambda', \tag{12}$$

where $\bar{\gamma}_{\lambda c}$ and $\bar{\gamma}_{\lambda' c'}$ represent the reduced width amplitudes and $\bar{E}_\lambda$ the pole positions in Park's alternative parametrization and $B_{\lambda c}$ and $B_{\lambda' c}$ are the newly introduced level-dependent boundary parameters, respectively.

Introducing the quantities $\mathcal{R}_{cc'}$ and $\mathcal{R}^B_{cc'}$ as

$$\mathcal{R}_{cc'} = \sum_{\lambda'\lambda}\bar{\gamma}_{\lambda' c'}\left(J^{-1}\right)_{\lambda'\lambda}\frac{1}{\bar{E}_\lambda - E}\bar{\gamma}_{\lambda c} \tag{13a}$$

$$\mathcal{R}^B_{cc'} = \sum_{\lambda'\lambda}\bar{\gamma}_{\lambda' c'}\left(J^{-1}\right)_{\lambda'\lambda}\frac{1}{\bar{E}_\lambda - E}\bar{\gamma}_{\lambda c}B_{\lambda c}, \tag{13b}$$

one finds an analogue expression to Eq. (3) for the wave function at the matching radius

$$u_{c'}(a'_c) = \sum_c \sqrt{\frac{\mu'_c a'_c}{\mu_c a_c}}\left(\mathcal{R}_{c'c}a_c\frac{du_c(r)}{dr} - \mathcal{R}^B_{c'c}u_c(a_c)\right)_{r=a_c}. \tag{14}$$

In order to enforce coinciding formal pole energies and cross section resonances, the level dependent boundary parameter is chosen to be the shift function at $E = \bar{E}_\lambda$,

$$B_{\lambda c} = S_c(\bar{E}_\lambda)\,. \tag{15}$$

The diagonal elements of J are constructed by a natural extrapolation to the diagonal case taking the limit $\bar{E}_{\lambda'} \rightarrow \bar{E}_\lambda$, which leads to

$$J_{\lambda\lambda} = 1 - \sum_c \bar{\gamma}^2_{\lambda c}\left.\frac{dS_c(E)}{dE}\right|_{E=\bar{E}_\lambda}. \tag{16}$$

Again, the collision matrix $\mathbf{U}$ can be expressed in terms of the new parametrization

$$\mathbf{U} = 2i\boldsymbol{\rho}^{\frac{1}{2}}\boldsymbol{O}^{-1}\left(\left[\mathbf{1} - \boldsymbol{\mathcal{R}}(\mathbf{S} + i\mathbf{P}) + \boldsymbol{\mathcal{R}}^{\boldsymbol{B}}\right]^{-1}\boldsymbol{\mathcal{R}}\right)\boldsymbol{\rho}^{\frac{1}{2}}\boldsymbol{O}^{-1} + \boldsymbol{I}\boldsymbol{O}^{-1}. \tag{17}$$

Similar to the Brune parametrization the enforced coincidence of R-matrix poles $\bar{E}_\lambda$ and observed resonance positions is beneficial to the parameter fitting process.

3 Implementation

3.1 First example

Park's alternative parametrization was implemented and integrated into the R-matrix module of GECCCOS. The new routine was tested with (n+^{16}O) scattering data. This is a challenging example due to the large number of resonances in this system. For the sake of simplicity the incident energy was restricted between 0 and about 4 MeV and only the total cross section and the (n,α) reaction cross section were taken into account. Preliminary results of a first fit for the total cross section and for the (n,α) reaction cross section can be seen in Fig. 1. In both cases a

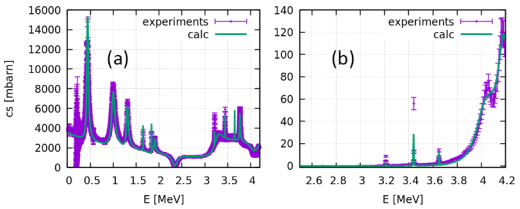

Figure 1. Preliminary fit of the n+^{16}O total cross section (a) and the angle integrated ^{16}O(n,α)^{13}C reaction cross section (b) using the Park's parametrization implemented in GECCCOS.

reasonable description of the data sets could be achieved where the coinciding R-matrix poles and cross section resonances vastly simplified the parameter fitting as expected.

3.2 Parameter reconstruction

The parametrizations of Park [2] and Brune [1] are very similar. They have the same pole energies and lead to the same non-diagonal values of $J_{\lambda\lambda'}$, Eq. (12), but differ in the diagonal elements, which are $J_{\lambda\lambda} = 1$ in Brune's parametrization instead of Eq. (16). Thus the corresponding reduced widths amplitudes satisfy the relation [2],

$$\tilde{\gamma}_{\lambda c} = (J_{\lambda\lambda})^{-1/2}\bar{\gamma}_{\lambda c}\,. \tag{18}$$

Comparing the expressions for the scattering matrix Eq. (6) and Eq. (17) one finds the identity

$$\mathbf{R} = \left[\mathbf{1} + \boldsymbol{\mathcal{R}}^{\boldsymbol{B}} - \boldsymbol{\mathcal{R}}\mathbf{B}\right]^{-1}\boldsymbol{\mathcal{R}}\,, \tag{19}$$

From Eq. (19) one realizes that the pole energies in the standard R-matrix paramaterization are given by the zero points of the determinant of $\left[\mathbf{1} + \boldsymbol{\mathcal{R}}^{\boldsymbol{B}} - \boldsymbol{\mathcal{R}}\mathbf{B}\right]$. Thus the shifted poles of the standard R-matrix can be directly extracted from the parametrizations of Park [2] and via an analogous relation also from the Brune [1] parametrization.

3.2.1 *Example*

For demonstration a single pole term with $J^\pi = 3/2^+$ was put in the n+^{16}O system with Park parameters $\bar{E}_\lambda = 3.7$ MeV, $\bar{\gamma}_{11} = 0.2$ and $\bar{\gamma}_{12} = 1.0$ with a matching radius of $a = 2.8$ fm. It can be seen in Fig. 2 that the position

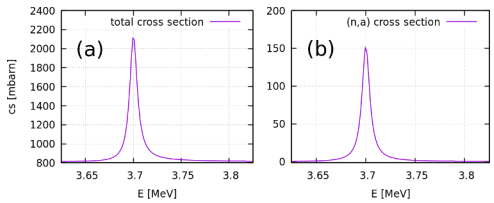

Figure 2. (a) n+^{16}O total cross section and (b) the corresponding ^{16}O(n,α)^{13}C reaction cross section with only one pole in the partial wave $J^\pi = 3/2^+$ with $\bar{E}_\lambda = 3.7$ MeV, $\bar{\gamma}_{11} = 0.2$ and $\bar{\gamma}_{12} = 1.0$ using Park's parametrization.

of the cross section resonance coincides with the R-matrix pole position in the total cross section as well as in the (n,α) reaction cross section.

Evaluating Eq. (19) with $\mathbf{B} = 0$ on a fine grid leads to the standard R-matrix element R_{11} displayed in Fig. 3. It clearly shows, as predicted by the zero point of the determinant, mentioned above, that the pole is shifted from 3.7 MeV to about 1.275 MeV in the standard R-matrix parametrization. Performing a parameter fit yields the γ-width amplitudes of the standard R-matrix, i.e. $\gamma_{11} = 0.199998387$ and $\gamma_{12} = 0.99999190$.

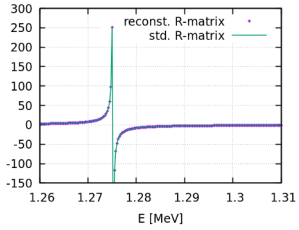

Figure 3. Pointwise reconstruction of the standard R-matrix element for the elastic channel in comparison with a calculation using the R-matrix parameters retrieved from fitting.

Although the standard parameters have not been transformed in closed form, the reconstruction yields excellent agreement with the obtained R-matrix values from Eq. (19). The cross sections calculated with the reconstructed standard R-matrix parameters show excellent agreement with those obtained from the original Park parameters (Fig. 4). An alternative method to determine the

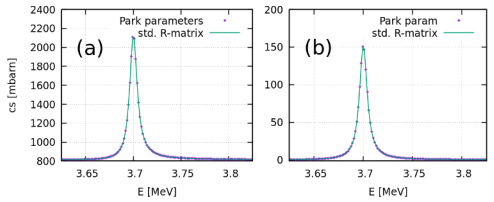

Figure 4. Cross sections obtained from original Park parameters in comparison with the corresponding reconstructed standard R-matrix parameters for (a) the total and (b) the (n,α) cross section.

standard R-matrix parameters associated with a given Park parametrization is a sequential approach, i.e. the transformation of $\bar{\gamma}$-values via Eq. (18) to Brune's $\tilde{\gamma}$-values (pole positions are the same) and subsequently use the procedure of Brune [1] to determine the corresponding standard R-matrix parameters.

4 Summary and Outlook

The two alternative R-matrix parametrizations, by Brune [1] and Park [2] were compared with the corresponding standard R-matrix parametrization. The big advantage of both is the simplified fitting process making the evaluation process much easier. Brune's parametrization generalized the transformation of R-matrix parameters under change of the boundary parameter. This leads to an R-matrix with pole positions coinciding with cross section resonances, but independent of B_c. Inspired by Brune, Park dropped orthonormality of the basis functions and introduced level-dependent boundary parameters to achieve the same. To test Park's parametrization it was implemented in the R-matrix module of GECCCOS and first test calculations were successfully performed in the (n+^{16}O) system. A scheme to reconstruct the standard R-matrix parameters from a given Park parametrization was proposed, implemented and successfully tested.

The implementation of the Brune parametrization into the R-matrix module of GECCCOS is in progress.

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