

R-matrix approach at the intersection with the statistical model regime

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Abstract. A hybrid R-matrix approach is proposed which combines the pole term decomposition of the R-matrix and a background R-matrix which is based on a coupled-channel pseudo-potential. The pseudo-potential is appropriately chosen in order to recover the observables obtained by the statistical model at the energy-onset of its validity. The additional pole terms describe the resonance structure at low energy not attainable in statistical model calculations. Due to its construction the hybrid method allows a smooth transition at the intersection with the statistical model regime. A new R-matrix code based on this hybrid approach was constructed. First applications to n-¹⁶O nuclear data between 0.2 and 5.0 MeV are very promising.

1. Introduction

R-matrix theory, originally proposed by Wigner and Eisenbud [1–3], is an elegant tool to describe resonant behaviour of cross sections without taking recourse to the complexity of the nuclear many-nucleon problem. In nuclear data evaluation for nuclei with mass number $A \geq 20$ R-matrix based approaches have been successfully applied for the description of experimentally measured reaction cross sections at low incident energies which usually exhibit many resolved resonances. At higher energies the measured reaction cross sections show only smooth energy dependences which are fairly well reproduced by statistical model calculations complemented by other bulk models, e.g. precompound or fission models [4]. Thus, evaluated data files of high quality can be generated for these nuclei.

For light nuclei ($A \leq 20$) these methods yield less satisfactory results. One reason is the lack of microscopic models which provide quantitatively reliable values of reaction cross sections. Another reason is the small level density of the involved compound nuclei which limits the applicability of the statistical model to rather high excitation energies. Because of the conceptual differences between the two approaches the continuous transition between the R-matrix regime and statistical model calculations represents a challenge and is not obvious. In addition one has also to manage requirements related with the extension of unitary R-matrix calculations up rather high energies.

In standard R-matrix codes a parametrization in terms of pole positions and associated widths parameters is used. In order to develop a procedure which guarantees continuity between the resonance regime and statistical model calculations, we must go beyond a phenomenological description and use the R-matrix formalism

as a tool for the solution of coupled-channels [5]. The corresponding theory is briefly sketched in Sect. 2 and implemented in our new R-matrix code which contains besides the standard resonance parameter representation of the R-matrix also a coupled-channel solver accounting for so-called pseudo-potentials, effective interactions depending on the relative coordinates of the relevant channels. The pseudo-potential approach should be sufficiently flexible to provide a fair description of statistical model calculations and simultaneously represents a proper basis for an extended R-matrix description. In Sect. 3 some details of the numerical implementation and first results on n-¹⁶O cross sections are discussed. A summary and a brief outlook is given in Sect. 4.

2. Theory basis

2.1. Concept of R-matrix

The key idea of R-matrix theory is the separation of the configuration space in an inner and an outer region. This idea by Wigner and Eisenbud [1–3] was elaborated by many authors, e.g. [5,6]. Assuming that the interaction in the outer region is known (vanishing potential or Coulomb potential) the wave function of the external region in channel c is known up to the corresponding S-matrix element for open and closed channels,

$$u_{c(c_0)}^{\text{ext}}(r) = \begin{cases} C_c [I_c(kr)\delta_{cc_0} - S_{cc_0}O_c(kr)] & \text{(open)} \\ A_{cc_0}W_{-\eta,l+\frac{1}{2}}(2\kappa_c r) & \text{(closed)}. \end{cases} \quad (1)$$

In Eq. (1) I_c and O_c are incoming and outgoing Coulomb functions, respectively, in case of open channels, $W_{-\eta,l+\frac{1}{2}}$ represents the Whittaker function in case of closed channels, the magnitudes C_c and A_{cc_0} are normalization constants.

The wave functions of the inner region reflect the effects of nuclear and Coulomb interactions on the

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relative motion and are usually unknown. Therefore the inner wave functions are described by a superposition of basisfunctions $\varphi_j(r)$ [3],

$$u_c^{\text{int}}(r) = \sum_{j=1}^N c_{cj} \varphi_j(r). \quad (2)$$

The coefficients c_{cj} in Eq. (2) provide the continuity of the logarithmic derivative at a given matching point $r = a$,

$$u_c^{\text{int}}(a) = u_{c(c_0)}^{\text{ext}}(a) \quad u_c^{\text{int}'}(a) = u_{c(c_0)}^{\text{ext}'}(a). \quad (3)$$

These conditions lead to the definition of the R-matrix for coupled-channels

$$u_c^{\text{int}}(r) = \sum_{c'} \sqrt{\frac{\mu_c}{\mu_{c'}}} R_{cc'}(E) [a u_{c'}'(a) - B_c u_{c'}(a)], \quad (4)$$

where μ_c represents the reduced mass in channel c and B_c is an arbitrary boundary parameter in channel c which does not affect the observables [5]. For our calculations we choose $B_c = 0$. However, another choice of B_c can be made if it is more appropriate.

2.2. The calculable R-matrix

In the following we briefly sketch the formalism of the calculable R-matrix following [5]. The starting point is the solution of the radial part of the coupled-channel Schrödinger equation within the inner region $0 \leq r \leq a$

$$[(T_c + E_c - E)\delta_{cc'} + V_{cc'}(r)] u_{c'(c_0)}(r) = 0, \quad (5)$$

where E_c is the threshold in channel c and $V_{cc'}$ the pseudo-potential. In these first considerations, non-orthogonality terms of the coupled-channel wave functions are neglected.

Due to the restriction of Eq. (5) to the inner region ($0 \leq r \leq a$) the Hamiltonian is not Hermitian [6]. The hermiticity can be restored by extending the Schrödinger equation with a surface term - the Bloch operator [7] \mathcal{L}

$$\mathcal{L} = \sum_c |c\rangle \mathcal{L}_c \langle c|, \quad (6)$$

with

$$\mathcal{L}_c = \frac{\hbar^2}{2\mu_c} \delta(r - a) \left(\frac{d}{dr} - \frac{B_c}{r} \right), \quad (7)$$

leading to the Bloch-Schrödinger equation

$$\sum_{c'} [T_c + \mathcal{L}_c + E_c - E]\delta_{cc'} + V_{cc'}] u_c^{\text{int}}(r) = \mathcal{L}_c u_c^{\text{ext}}(r). \quad (8)$$

The wave functions of inner and outer region are separated as can be easily seen from Eq. (8).

The multi-channel R-matrix $R_{cc'}(E)$ can be written as

$$R_{cc'}(E) = \frac{\hbar^2}{2\sqrt{\mu_c \mu_{c'}} a} \sum_{i,i'=1}^N \varphi_i(a) (C^{-1})_{ci,c'i'} \varphi_{i'}(a), \quad (9)$$

where $C_{ci,c'i'}$ are the matrix elements of the Hamiltonian,

$$C_{ci,c'i'} = \langle \varphi_i | T_c + \mathcal{L}_c + E_c - E | \varphi_{i'} \rangle \delta_{cc'} + \langle \varphi_i | V_{cc'} | \varphi_{i'} \rangle. \quad (10)$$

Because of hermiticity a spectral decomposition of the R-matrix can be formulated

$$R_{cc'}(E) = \sum_n \frac{\gamma_{nc} \gamma_{nc'}}{E_n - E}, \quad (11)$$

where the real poles E_n are the eigenvalues of the matrix $C(E)$ at $E = 0$ and the reduced width-amplitudes γ_{nc} of a pole E_n in channel c are expressed as a function of the corresponding normed eigenvectors v_n ,

$$\gamma_{nc} = \left(\frac{\hbar^2}{2\mu_c a} \right)^{1/2} \sum_{i=1}^N v_{n,ci} \varphi_i(a). \quad (12)$$

The dimension of the matrix C is equal to the product of the number of channels by the number of basis functions N .

The scattering matrix S can be directly obtained from the R-matrix with

$$S = Z_0^{-1} Z_1, \quad (13)$$

with the matrix elements of Z_0 and Z_1 given by

$$Z_{0cc'} = (k_{c'} a)^{-1/2} [O_c(k_c a) \delta_{cc'} - k_{c'} a R_{cc'} O_{c'}'(k_{c'} a)] \quad (14a)$$

and

$$Z_{1cc'} = (k_{c'} a)^{-1/2} [O_c(k_c a) \delta_{cc'} - k_{c'} a R_{cc'} I_{c'}'(k_{c'} a)]. \quad (14b)$$

It is important to point out that the dimension of the R-matrix is equal to the number of all channels, whereas the dimension of the scattering matrix is equal to the number of open channels. Hence the dimension of the R-matrix is constant for all energies while the dimension of the scattering matrix might vary with energy.

From the knowledge of the S-matrix it is possible to calculate the scattering amplitude allowing to determine all observables (e.g. [5]).

2.3. The phenomenological R-matrix

Following [1-3,5] it becomes obvious that the R-matrix is essentially the inverse logarithmic derivative at the matching radius a . The phenomenological approach makes direct use of Eq. (11) adjusting the reduced widths γ_{nc} and poles E_n to experimental data.

In practice this yields a very good description of experimental cross sections, but cannot provide predictions. Because no information about the microscopic Hamiltonian is considered the physical interpretation is also limited.

2.4. Hybrid approach and pseudo-potential

Standard R-matrix codes use the spectral decomposition of Eq. (11) considering the pole positions E_n and associated widths γ_{nc} as parameters. Due to the lack of a reliable microscopic procedure for the determination of E_n and the widths γ_{nc} these quantities have to be adjusted in order to reproduce experimental data. In the calculable R-matrix the number of pole terms is large (number of channels \times number of basis functions), but only few poles lead to obvious resonances in the observables, while remaining poles constitute the background interaction.

Therefore, phenomenological R-matrix approaches use only the minimal number of poles and describe the background with few so-called shadow poles. In addition simplifications are applied which provide a more direct relation to the S-matrix and thus to the observables. In most cases this leads to an excellent agreement with experimental data. However, due to the lack of a microscopic basis predictions and physics interpretations, e.g. identification of true many-body effects, are not possible. The latter is of importance with regard to the transition between the resonance regime and statistical model calculations.

In order to guarantee a smooth transition between the two regimes the observables from the statistical model calculation are considered to be generated by a coupled-channel pseudo-potential $V_{cc'}$. Thus the pseudo-potential represents an effective interaction obtained via projection of the microscopic many-body interaction onto channel states. The pseudo-potential $V_{cc'}$ is in principle non-local and depends on the relative coordinates of the channels c and c' . As an effective potential it is frequently assumed to be local [5] which simplifies the coupled-channel calculations. In this work the assumption is even more justified since the statistical model relies on a completely different concept and the pseudo-potential $V_{cc'}$ cannot be derived microscopically and provides only an effective description. Nevertheless it can be expected to be a smooth function of r because the channel thresholds E_c are already contained in Eq. (8). Hence a parametrized form of the pseudo-potential has to be assumed whose parameters have to be adjusted to reproduce the observables obtained via statistical model calculations.

The determination of the R-matrix starts from solving the Bloch-Schrödinger Eq. (8) with the pseudo-potential included. With proper basis functions $\varphi_i(r)$ one obtains from Eq. (10) the matrix C and thus the R-matrix $R_{cc'}^{bg}(E)$ via Eq. (9). In order to describe experimental observables we use $R_{cc'}^{bg}(E)$ as a background R-matrix and add pole terms

$$R_{cc'}(E) = R_{cc'}^{bg}(E) + \sum_m \frac{\gamma_{mc}\gamma_{m'c'}}{E_m - E}. \quad (15)$$

The poles E_m and the associated reduced widths γ_{mc} have to be adjusted in order to reproduce the resonances of the experimental cross sections which cannot be described within the statistical model. In general it is expected that the γ_{nc} are small and the poles E_m lie within the energy region of observed resonances. Thus the effect of additional pole terms will be negligible in the statistical model regime. Thus the ansatz Eq. (15) should guarantee a continuous transition between R-matrix and statistical model regimes. Because the background R-matrix, $R_{cc'}^{bg}(E)$, is optimized for reproducing statistical model calculations. In addition, the additional pole terms will reflect the many-nucleon structure of the compound nucleus, while $R_{cc'}^{bg}(E)$ accounts for bulk contributions.

3. Implementation and results

For the application of the hybrid approach a new R-matrix code was developed which includes the standard spectral decomposition of the phenomenological R-matrix as well as the determination of a background R-matrix within the coupled-channel formalism. For the solution of

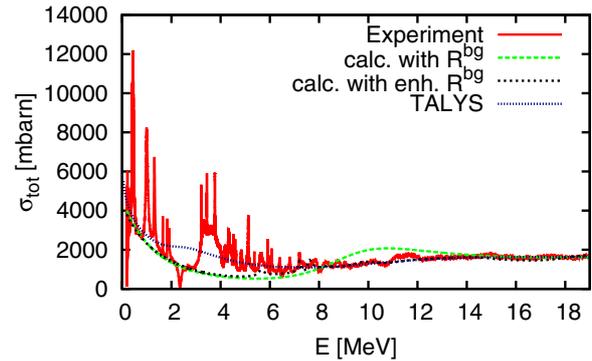


Figure 1. Experimental total cross section in comparison with the cross sections obtained from background R-matrix spectrum, the modified background spectrum and a statistical model TALYS calculation.

the coupled Bloch-Schrödinger equation (8) the Lagrange mesh technique [5] was applied. The use of Lagrange functions for $\varphi_i(r)$ simplifies the determination of the matrix C significantly. However, the determination of the eigenvalues E_n and eigenvectors v_{nc} is still a bottleneck due to the high number of dimensions (number of channels \times number of basis functions) in matrix C . The number of channels is also rising with increasing energy and requiring large scale computing capabilities.

The optimization of the parameters of the hybrid approach (E_n , γ_{nc} and the background potential) is performed by the DAKOTA package [8].

3.1. Example: Neutron-induced reaction on ^{16}O

The hybrid approach is particularly well suited for light nuclei. For a first test of the hybrid approach we chose neutron-induced reactions on ^{16}O which is a system of great interest at present. As a first guess of the pseudo-potential we use the real part of the Woods-Saxon shaped volume term taking the parameters from the RIPL-3 library [9]. Slight optimization of the Woods-Saxon parameters already reproduced some of the basic cross section structure as can be seen in Fig. 1. An imperfection shows up at about 10 MeV where the cross section has a slight bump.

All poles with different J^π but the same l are identical because the only angular momentum dependence of the Hamiltonian is in the centrifugal term of the kinetic energy operator. Varying the positions and widths of the poles in the relevant region from 0–10 MeV, as illustrated in Fig. 2, the bump at 10 MeV can be healed. This indicates the necessity of some J -dependence of the background pseudo-potential.

In order to show the transition to the statistical model regime we performed calculations with the TALYS code [10]. As one can see in Fig. 1 our background R-matrix calculation coincides nicely with the experimental data and the statistical model calculation beyond 14 MeV.

The resonance structure of the cross section can be reproduced by adding pole terms to the background R-matrix (Eq. (15)), displayed in Fig. 3. Within the range from 0.2–5 MeV the resonance structure is nicely reproduced while a physically reasonable matching radius of $a = 7$ fm is kept.

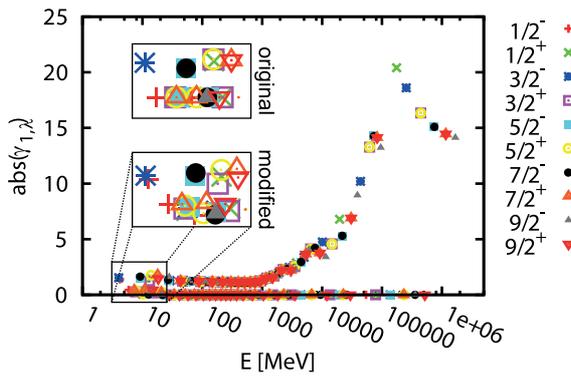


Figure 2. Positions of background poles and the absolute value of their corresponding widths for various partial waves for the original spectrum obtained from pseudo-potential and the modified spectrum.

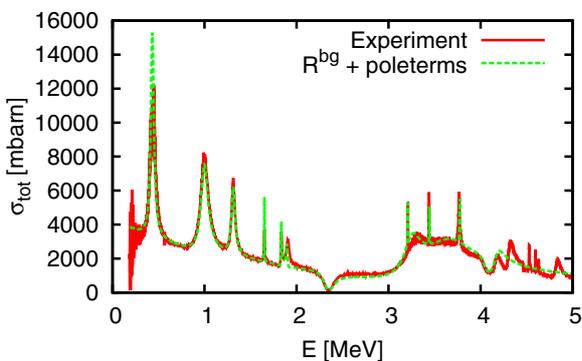


Figure 3. Experimental total cross section in comparison with cross section obtained by the hybrid R-matrix approach (background spectrum + additional pole terms).

4. Summary and outlook

The presented hybrid approach which combines a background spectrum obtained from a coupled-channel calculation with additional pole terms seems very promising. The background potential was able to reproduce the basic structure of the total cross section at energies beyond 13 MeV using a physically reasonable matching radius of 7 fm. With additional pole terms the resonance structure from 0.2–5 MeV could be reproduced. Yet the fit is not perfect and is more to be seen as a proof of concept. Furthermore when going to higher energies more channels have to be included leading to more parameters. Interference effects and nonlinearity effects raise the demand for versatile fitting routines.

The proper parametrization of the background potential has shown to be crucial for the shape of the basic cross section structure. Our studies clearly show the necessity of a J-dependent background potential. The required modifications in the background spectrum were small and therefore the corresponding effect on the pseudo-potential will be extracted via perturbative methods.

The contributions of the (n,γ) channel were negligible. In the transition region starting at about 13 MeV, 3-body reactions will play an important role. The proper inclusion of (n,γ) and 3-body processes in our R-matrix code is currently work in progress.

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References

- [1] E.P. Wigner, Phys. Rev. **70**, 15 (1946)
- [2] E.P. Wigner, Phys. Rev. **70**, 606 (1946)
- [3] E.P. Wigner, L. Eisenbud, Phys. Rev. **72**, 29 (1947)
- [4] A. Koning, E. Bauge, C. Dean, E. Dupont, U. Fischer, R. Forrest, R. Jacqmin, H. Leeb, M. Kellett, R. Mills et al., Journal of the Korean Physical Society **59/2**, 1057 (2011)
- [5] P. Descouvemont, D. Baye, Reports on Progress in Physics **73**, 036301 (2010)
- [6] A.M. Lane, R.G. Thomas, Rev. Mod. Phys. **30**, 257 (1958)
- [7] C. Bloch, Nucl. Phys. **4**, 503 (1957)
- [8] B. Adams, L. Bauman, W. Bohnhoff, K. Dalbey, M. Ebeida, J. Eddy, M. Eldred, P. Hough, K. Hu, J. Jakeman et al., *DAKOTA, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 5.4 User's Manual*, Sandia Technical Report SAND2010-2183 (2009), updated April (2013)
- [9] R. Capote, M. Herman, P. Obložinský, P. Young, S. Goriely, T. Belgya, A. Ignatyuk, A. Koning, S. Hilaire, V. Plujko et al., Nuclear Data Sheets **110**, 3107 (2009)
- [10] A. Koning, S. Hilaire, S. Goriely, *TALYS – A nuclear reaction program* (2015), <http://www.talys.eu/home/>