Introduction to neutron-induced reactions and the *R*-matrix formalism

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Introduction

One of the most striking features of neutron-nucleus interactions is the resonance structure observed in the reaction cross sections at low incident neutron energies. Since the electrically neutral neutron has no Coulomb barrier to overcome, and has a negligible interaction with the electrons in matter, it can directly penetrate and interact with the atomic nucleus, even at very low kinetic energies in the order of electron-volts.

The cross sections can show variations of several orders of magnitude on an energy scale of only a few eV. The origin of the resonances is well understood: they are related to the excitation of nuclear states in the compound nuclear system formed by the neutron and the target nucleus, at excitation energies lying above the neutron binding energy of typically several MeV. The average distance between the resonances reflect the density of nuclear levels. Typical neutron-induced total cross sections for several masses are shown in figure 1. From the figure one can observe an decreasing level spacing with increasing mass. This is a general trend observed in cross section data, with an exception near closed shell nuclei where the level spacing becomes much larger, or equivalently the level density much smaller, as shown in the figure for the nucleus ^{208}Pb.

The compound nucleus model was introduced by Niels Bohr to explain the observed resonances in neutron-nucleus reactions. The wavelength of low energy neutrons is comparable to the size of the nucleus. Typical widths Γ of measured resonances are in the order of electron-volts. According to Heisenberg's uncertainty principle, the corresponding life time of the compound nucleus is in the order of $\tau = \hbar/\Gamma \simeq 10^{-15}$ s, several orders of magnitude larger than the typical time needed by a neutron to cross a nucleus without interaction. In this

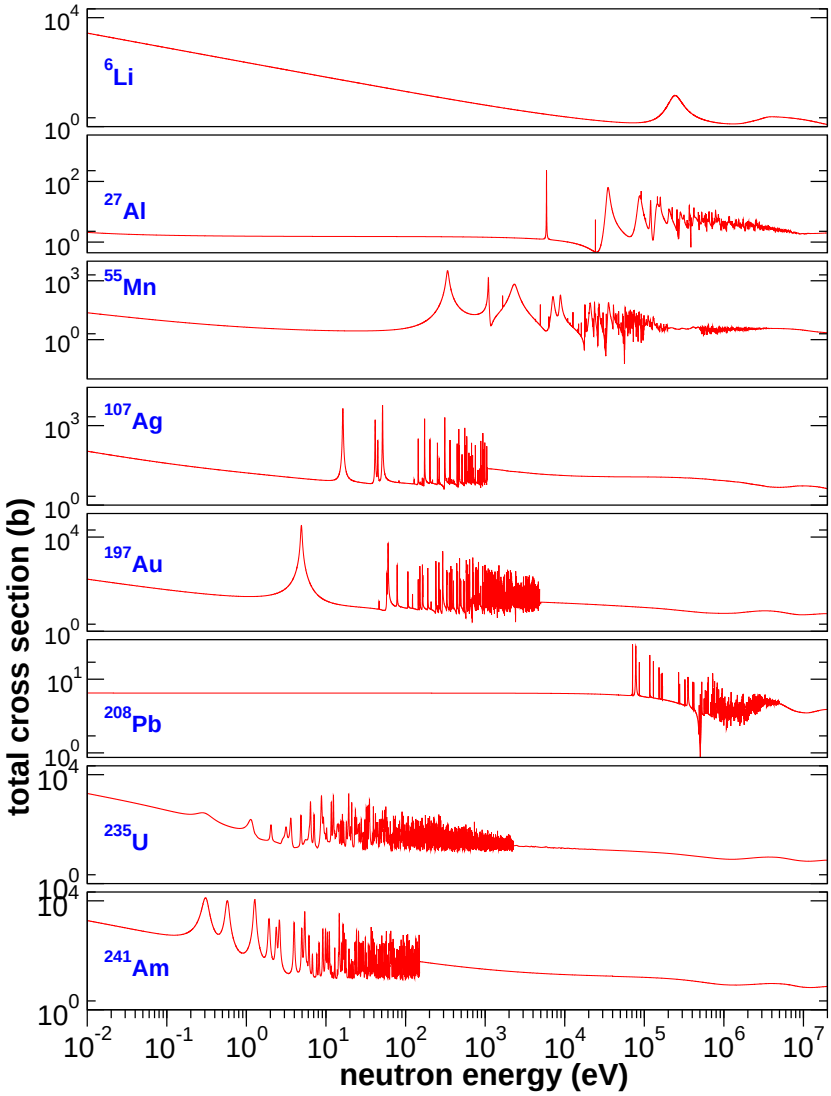

Figure 1: The neutron total cross section of several nuclei showing large differences in the resonance spacings.

picture, the neutron binding energy which becomes available to the compound nucleus, is rearranged among all nucleons, and gives rise to a complex configuration corresponding to a well defined nuclear state with an energy, spin and parity. Within Fermi's description of excitations of particle-hole configurations, such a state would correspond to an extremely complicated configuration of a many particle, many hole state. The compound nucleus may then decay through the energetically allowed channels. The way of decay and the decay probability of the compound nucleus is considered to be independent from the way how the compound nucleus was formed, but respecting conservation of energy and angular momentum. The decay probability is equal to the branching ratio Γ_x/Γ

where Γ_x is the width related to the decay by emission of a particle x, which at low energy is mainly a gamma ray or a neutron.

In direct reactions, as the opposite reaction mechanism to compound nucleus reactions, the incident neutron interacts directly with one or a few nucleons without forming a compound nucleus. The time scale of direct reactions is in the order of 10^{-22} s and much shorter than compound-nucleus resonance reactions. Direct reactions become important for the heavier nuclei at neutron energies higher than about 10 MeV where the De Broglie wavelength of the neutron becomes comparable to the size of nucleons. But also at lower neutron energies, mainly for light A or closed shell nuclei, direct reactions may contribute significantly to the total reaction cross section. In general for neutrons with energies below 1 MeV the here discussed compound nucleus reactions prevail.

In figure 2 a picture of the compound nucleus reaction is sketched. After the formation of the highly excited state by an incident neutron, the compound nucleus can decay by emission of gamma radiation, which is called radiative neutron capture, or by by emission of a neutron, which is elastic scattering. If the kinetic energy of the neutron is high enough, threshold reactions are possible, like inelastic scattering, leaving the target nucleus in an excited state. If the excitation energy is higher than the fission threshold, fission is energetically allowed. Due to the pairing effect, the neutron binding energy for even compound nuclei is considerably lower than for odd compound nuclei, which for some of the heavy nuclei results in a fissionable nucleus even if the incident neutron has nearly zero kinetic energy. All these reactions show resonances at the same energies corresponding to the excitation of the nuclear levels in the compound nucleus. The shapes of the resonances are different and related to the involved widths.

The possible neutron-nucleus reactions vary with incident neutron energy. The nuclear reaction that is always present if a reaction is energetically allowed is elastic scattering. This may be scattering from the nuclear potential, also called shape elastic or sometimes hard sphere scattering, without forming a compound nucleus. In addition resonant elastic scattering through a compound nucleus may be present. The potential scattering is a smooth and nearly energy independent cross section as a function of energy but interferes with the resonant scattering cross section.

The widths of isolated resonances in reaction cross sections have in good approximation a familiar Breit-Wigner shape. The time dependence of the wave function $\Psi(t)$ of a non-stationary state at E_0 with a life time $\tau = \hbar/\Gamma$, is observed as an exponential decay in time. The squared absolute value of the Fourier transform of $\Psi(t)$ gives the energy distribution $P(E)$ having the Breit-Wigner form

$$P(E) = \frac{\Gamma/2\pi}{(E - E_0)^2 + \Gamma^2/4} \tag{1}$$

which is the typical shape for any quantum-mechanical state with a finite lifetime. .

In the limiting case of a single, isolated $\ell = 0$ resonance at low energy E_0 and with capture, fission and elastic scattering as the only open channels, the total cross section can be expressed in the single level Breit-Wigner form as

$$\sigma_T(E) = 4\pi R'^2 + \pi\lambda\!\!\!^{-2} g \left(\frac{4\Gamma_n (E - E_0) R'/\lambda\!\!\!^{-} + \Gamma_n^2 + \Gamma_n\Gamma_\gamma + \Gamma_n\Gamma_f}{(E - E_0)^2 + (\Gamma_n + \Gamma_\gamma + \Gamma_f +)^2/4} \right) \qquad (2)$$

where Γ_n is the neutron width, Γ_γ the radiative width, Γ_f the fission width, g the statistical spin factor and $\lambda\!\!\!^{-}$ the reduced de Broglie wave length of the neutron. The first term in the sum is the potential scattering cross section $\sigma_p = 4\pi R'^2$, where R' is the effective nuclear radius, with a value close to the channel radius a. the Full R-matrix expressions for the cross sections are given later.

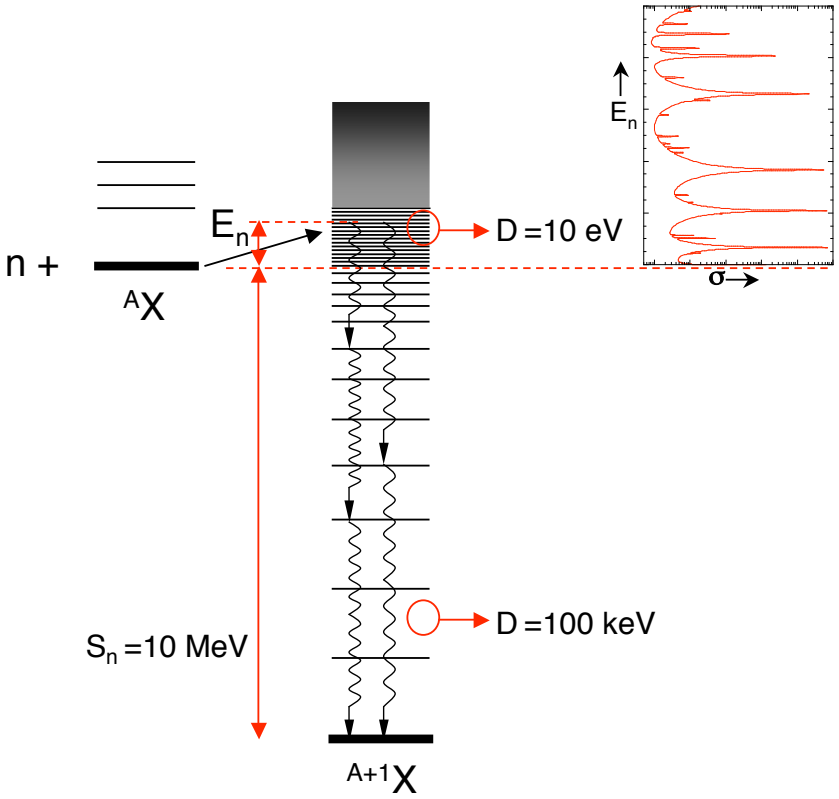

Figure 2: Schematic view of the formation and decay of a compound nucleus. Orders of magnitude of the level spacing and the neutron separation energy for a heavy mass nucleus are shown. The resonances observed in reaction cross sections, shown in the upper right part, correspond to the excitation of nuclear levels.

At the high excitation energies above the neutron binding energies, for most nuclei the nuclear system is extremely complex and no nuclear model is capable of predicting the position and other properties of these excited states. Cross sections can therefore be accessed only by measurements. For a heavy nucleus the wave function describing such a highly excited state may have as much as 10^6 components. Also the level density in this region is consequently very high. A neighbouring eigenstate can be excited by only a small change in excitation energy and may have a completely different wave function. This is a manifestation of what is also called chaotic behaviour. Due to extreme configuration mixing, the nucleus in this regime above the neutron threshold has a statistical behaviour. This is expressed by the assumption that the matrix elements relating nuclear states have a random character, governed by a Gaussian distribution with zero mean. This statistical model of the compound nucleus is referred to as the Gaussian Orthogonal Ensemble (GOE) [1–5].

The statistical model has direct consequences on the observables of the reaction cross sections. The channel widths are proportional to the square of the matrix elements and have therefore a chi-squared distribution with one degree of freedom. also called the Porter-Thomas distribution [6]. The observed gamma width of a resonance is the sum of many, for medium and heavy nuclei several tens of thousand, individual gamma widths and tends therefore more to a Gaussian distribution. Observed fission widths correspond to a relatively small number of fission channels, at maximum three or four. The resulting distribution can be approximated by an effective chi-squared distribution with a small, fractional number of degrees of freedom [7].

With increasing excitation energy the widths of the states start to overlap and the resulting cross sections become smooth. The properties of the eigenstates, like the decay widths, fluctuating from one state to another, become apparent as values averaged over many resonances. These average values on the contrary can be predicted by nuclear models, parametrized with average properties. Measured average cross sections can therefore finetune the parametrization of these models.

At even higher excitation energies, many more decay channels open up and cross section measurements become very difficult or impossible. Reaction cross sections may therefore only be accessible by nuclear model calculations.

As an example, in figure 3 the neutron capture cross section of ^{238}U is shown on an energy scale spanning more than ten decades. The resonance structures, given by resonance paramters, are clearly visible in the low energy part while the smooth cross section at higher energies is parametrized in the libraries by interpolation tables. The sudden transition between these two regimes is therefore not physical but related to these different descriptions.

In order to appreciate the importance of the cross sections at different energies,

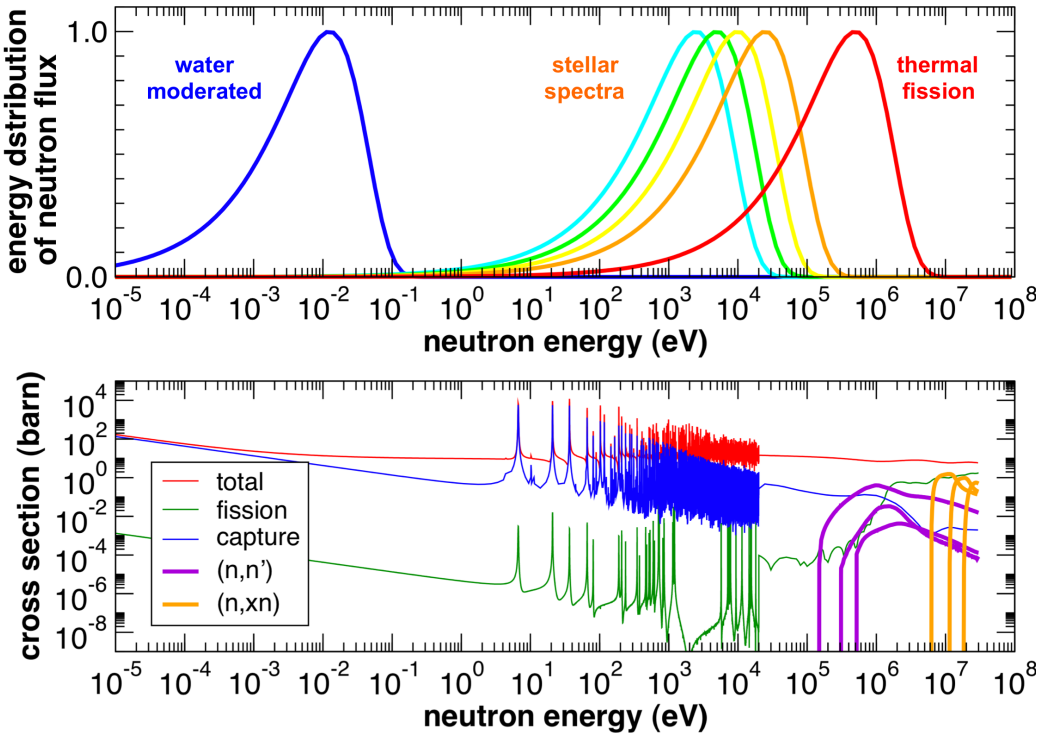

Figure 3: The neutron capture cross section of ^{238}U together with several different neutron source energy distributions in a wide energy range.

typical energy distributions of neutron fluxes are also shown in the figure. The energy region around a few tens of meV is called the thermal region and is of importance in reactor physics where the by water moderated neutrons are in thermal equilibrium with the water and have Maxwell-Boltzmann distributed velocities peaked at an equivalent kinetic energy $k_B T$. For a temperature of nearly 300 K this corresponds to 25.3 meV or a velocity of 2200 m/s. The thermal cross section at 25.3 meV is an important quantity and can be measured accurately with only small amounts of material in reactor experiments.

A different energy distribution is found for neutrons in certain stars and responsible for the synthesis of the isotopes heavier than about $A = 60$ in the universe. The neutrons are present as a hot gas and also have a Maxwellian kinetic energy distribution but now at temperatures with $k_B T$ ranging from 5 to 100 keV. Stellar nucleosynthesis will be briefly outlined later.

Several distribution functions describe in a satisfactory way the kinetic energy distribution of neutrons from the nuclear fission process. The neutrons from ^{235}U thermal neutron induced fission follow well a Maxwellian kinetic energy distribution, peaked at about 1 MeV. This distribution is also shown in figure 3.

In the resolved resonance region, which includes the thermal region, the reaction cross sections can be rigorously described in terms of resonance parameters, which are the properties of the excited states like energy, spin and parity. This is done by means of *R*-matrix theory, which is outlined in more detail in a next section. The advantage of the parametrization of resonant cross sections by the *R*-matrix formalism is that relatively few data are needed from which Doppler broadened cross sections at any temperature can be calculated.

The *R*-matrix description can be extended to the unresolved resonance region, where average resonance parameters can be adjusted to describe the cross sections. A related approach in this energy region and at higher energies is the use of optical model calculations. The interaction with the nucleus is then modelled by a complex potential well. By solving the Schrödinger equation one can calculate the cross sections. The difficulty lies in the parametrization of the potential.

Neutron induced reaction data are of great importance for nuclear reactor physics. In several other fields, including astrophysics and fundamental symmetries, neutron induced reactions play also an important role. Some items will be discussed in the following sections. In addition, important information on level densities, a key ingredient in many nuclear reaction codes, can be obtained directly from neutron resonance spectroscopy [8]. Many of the experimental data have been compiled [9–13] and once evaluated, made available through nuclear data libraries like BROND [14], ENDF-B [15], JEFF [16] and JENDL [17] and CENDL [18].

1 The *R*-matrix formalism

If the wave functions of the nuclear system before and after the reaction were known, one could calculate the cross section with the usual concepts of reaction theory. While the incoming waves are known, the reaction modifies the outgoing wave functions in a generally unknown way.

The idea behind the *R*-matrix formalism is to use the wave function of the nuclear system of two particles when they are so close that they form a compound nucleus. Although the wave function of the compound nucleus is extremely complicated, one can expand it in its eigenstates. Matching then the incoming and outgoing waves to the internal wave function provides a way to describe the cross section of the reaction in terms of the properties of the eigenstates of the compound nucleus. These properties are basically the energy, spin, parity, and a set of partial widths related to the widths of the decay modes of the compound nucleus.

This method of describing a reaction cross section using only the properties of nuclear excitation levels, is at the same time also the most important limitation. No information of the forces inside the nucleus is needed or can be extracted. The

nucleus is treated as a black box of which the properties of the eigenstates have to be measured in order to describe the cross sections.

The binary nuclear reactions proceeding from one system of two particles to another system of two particles can be described with the general R-matrix theory. For neutron induced reactions, but also in other cases, such a reaction goes often through the formation of a compound nucleus X^*.

$$A + a \rightarrow X^* \rightarrow B + b \tag{3}$$

The R-matrix formalism does not only apply to compound nucleus reactions. Both direct and indirect reactions can be described with it. The inclusion of the Coulomb interaction allows us to use it also for charged particle reactions. But the theory is applicable only in a general way for binary reactions which is appropriate for neutron induced reactions up to energies of several tens of MeV.

In a very general way, the cross section of a two-body nuclear reaction could be calculated if the nuclear wave functions were known. The wave functions could be calculated by solving the Schrödinger equation for the nuclear system. This requires that the nuclear potential is known. When the two particles are far away, the interaction can be considered absent for neutral particles or to be the Coulomb interaction for charged particles. In these cases it is indeed possible to calculate the wave functions.

When the two particles are so close to each other that a nuclear reaction takes place, the potential of the interaction is extremely complicated. For certain energy ranges and reactions this potential can still be approximated or calculated [19] and the wave functions and cross sections can be calculated. In other cases however, and especially in the resolved resonance region, the complexity of the reacting system does not allow this.

The first step is to consider that the reaction process can be split up geometrically into two regions for each channel where a channel is the precise constellation of particles and their spins. If the separation is smaller than the channel radius a_c, all nucleons involved in the reaction are close to each other and form a compound nucleus. Although the wave function of the compound nucleus is extremely complicated, it can be expanded as a linear combination of its eigenstates without solving explicitly the Schrödinger equation of the system. In the external region, at distances larger than a_c, the potential is zero for neutral particles or is the Coulomb interaction for charged particles and the Schrödinger equation of the system can be solved. The properties of the eigenstates of the compound nucleus are included in the R-matrix. Equating the values and derivatives of the wave functions at the boundary of the internal and external region assures a smooth wave function and the cross sections can be calculated. The exact internal wave function is not needed, only the values and derivatives at the nuclear surface.

In the following we describe in more detail the *R*-matrix formalism which links the properties of the nuclear states to the cross sections. The cross section in the thermal energy region is also described by the *R*-matrix formalism. Reaction cross sections at thermal energy are the sum of the contributions of all nuclear states, i. e. the resonances but also the bound states, sometimes referred to as "negative energy" resonances. Other reaction formalisms have been used in the past, like the *K*-matrix formalism [20] still in use for particle physics [21], but for neutron-induced resonance reactions the *R*-matrix formalism, and in particular one of its approximations, is nowadays the preferred formalism.

The *R*-matrix formalism was first introduced by Wigner and Eisenbud [22]. A most extensive and detailed overview has been given by Lane and Thomas [23] and by Lynn [1]. More recently, Fröhner [24] summarized the *R*-matrix formalism together with other useful considerations on nuclear data evaluation. Other related references of interest can be found elsewhere [25–35]. A brief outline of the formalism will be given in order to understand its basic principles.

1.1 Channel representation

It is customary to use the concept of channels in the description of nuclear reactions, which will be limited to two particle reactions in the following. The entrance channel c consists of a particular initial constellation of particles and all the quantum numbers necessary to describe the corresponding partial wave function. The type of the two particles α_1 and α_2, with their spins I_{α_1} and I_{α_2}, and their states of internal excitation are denoted by α. Four quantum numbers are needed to include the spins of the particles in a channel. The most appropriate combination is the orbital angular momentum ℓ, the channel spin j, which is the combined spin of the two particles

$$\mathbf{j} = \mathbf{I}_{\alpha_1} + \mathbf{I}_{\alpha_2}\,, \tag{4}$$

the total angular momentum J

$$\mathbf{J} = \mathbf{j} + \ell \tag{5}$$

and its projection on the z-axis m_J. So the entrance channel c can be designated by the set

$$c = \{\alpha, \ell, j, J, m_J\} \tag{6}$$

Similarly, the exit channel is given by

$$c' = \{\alpha', \ell', j', J', m'_J\} \tag{7}$$

The reaction $\alpha \rightarrow \alpha'$ may go through the formation of a compound nucleus, like often the case with neutron induced reactions. The reaction can then be written as $\alpha \rightarrow A^* \rightarrow \alpha'$. The spin and parity are of course conserved in all stages of the reaction and the compound nucleus has its defined spin J and parity π. The

conservation of spin and parity puts restrictions on the entrance channels that are open to form the compound nucleus or the exit channels open for the decay of the compound nucleus. For neutrons and protons the intrinsic spin is $1/2$ and the intrinsic parity is positive. Conservation of angular momentum gives the vector addition:

$$\mathbf{J} = \mathbf{I}_{\alpha_1} + \mathbf{I}_{\alpha_2} + \ell = \mathbf{I}_{\alpha'_1} + \mathbf{I}_{\alpha'_2} + \ell' \tag{8}$$

and conservation of parity gives, using $+1$ for positive and -1 for negative parity:

$$\pi = \pi_{I_{\alpha_1}} \times \pi_{I_{\alpha_2}} \times (-1)^{\ell} = \pi_{I_{\alpha'_1}} \times \pi_{I_{\alpha'_2}} \times (-1)^{\ell'} \tag{9}$$

The conservation of angular momentum has important consequences for cross section calculations based on channels. The total number of possible combinations to sum the spins and orbital momentum is $(2I_{\alpha_1}+1)(2I_{\alpha_2}+1)(2\ell+1)$. Only $2J+1$ orientations of them add up to J. For this reason in expressions for cross sections of the formation of a compound nucleus level with spin J for a given ℓ the statistical factor $g(J)$

$$g(J) = \frac{2J+1}{(2I_{\alpha_1}+1)(2I_{\alpha_2}+1)} \tag{10}$$

is taken into account.

The boundary $r = a_c$ is the limit between the internal region, where all the nucleons interact, and the external region where the incident and target particles do not have a nuclear interaction, other than possibly a Coulomb interaction. Although there is no sharp limit, in practice the channel radius a_c can be taken just slightly larger than the radius $R' = R_0 A^{1/3}$ of a spherical nuclear volume with $A = A_{\alpha_1} + A_{\alpha_2}$ nucleons, and where for R_0 usually the value 1.35 fm is used. This scattering radius can be used as a first approximation of the low-energy potential scattering cross section σ_{pot} with the relation

$$\sigma_{\text{pot}} = 4\pi R'^2 \tag{11}$$

Experimental values of R' show larger structures around the smooth curve $R' = R_0 A^{1/3}$ which can be well described with optical model calculations. In evaluated nuclear libraries the channel radius a_c can be defined to have either the numerical value of a possibly energy-dependent scattering radius R', or an energy-independent, mass-dependent channel radius given by

$$a_c = 0.8 + 1.23 A'^{1/3} \text{ fm} \tag{12}$$

where A' is the ratio of the isotope mass to the mass of the neutron. The channel is defined in the center of mass and the reduced mass of the particles is

$$m_c = m_\alpha = \frac{m_{\alpha_1} m_{\alpha_2}}{m_{\alpha_1} + m_{\alpha_2}} \tag{13}$$

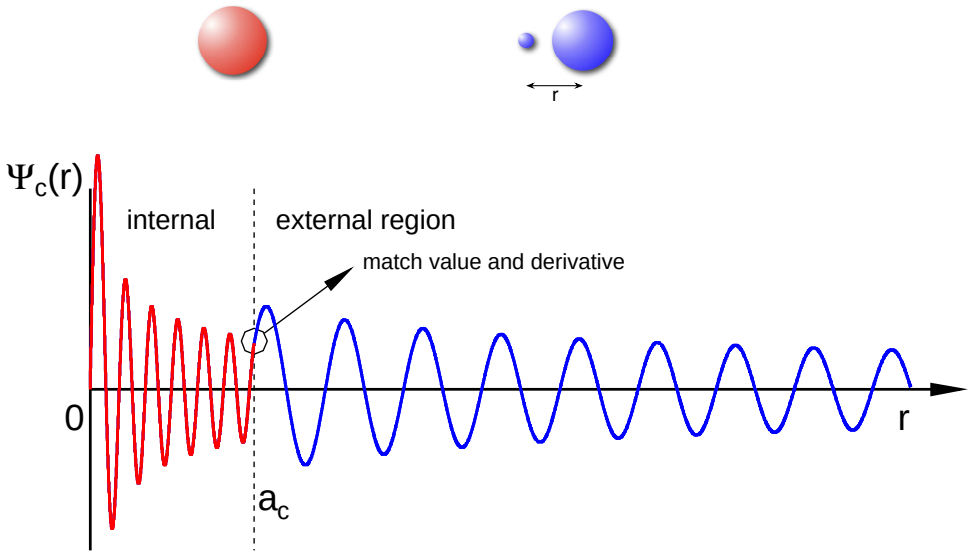

Figure 4: Schematic view of the wave function of a channel as a function of the separation distance r. The wave function in the internal region $r < a_c$ is an expansion of the eigenstates of the compound nucleus. The full internal ($r < a_c$) wave function is not needed, only the value and derivative at $r = a_c$ where it matches the known external ($r > a_c$) wave function which is related to the Bessel functions.

and the wave number k, related to the de Broglie wavelength λ, is

$$k_c = k_\alpha = \frac{1}{\lambda_c} = \sqrt{\frac{2m_\alpha E_\alpha}{\hbar^2}} \tag{14}$$

and the relative velocity is

$$v_c = v_\alpha = \hbar k_c / m_c \tag{15}$$

The dimensionless distance ρ_c is used to indicate the distance r_c in measures of de Broglie wavelengths.

$$\rho_c = \rho_\alpha = k_c r_c \tag{16}$$

1.2 The wave function in the external region

The system of the two particles interacting through a central potential $V(r)$ can be described by the Schrödinger equation of the motion of the reduced mass particle. Also, using spherical coordinates, the solution $\psi(r,\theta,\phi)$ can, in case of a central potential, be separated in a radial and an angular part

$$\psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi) \tag{17}$$

The radial part $R(r)$ although still depends on the non-negative integer solutions $\ell(\ell+1)$ of $\Theta(\theta)$. The integers appearing in the solution of $\Phi(\phi)$ are $m_\ell = 0, \pm 1, \pm 2 \ldots \pm \ell$. The solutions of the angular part $\Theta(\theta)\Phi(\phi)$ do not depend on the central potential and are the spherical harmonics $Y^\ell_{m_\ell}(\theta,\phi)$. Only the solution $R(r)$ of the radial part depends on the potential $V(r)$. The radial Schrödinger equation

$$\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - \frac{2m_c}{\hbar^2}(V(r)-E)\right] R(r) = 0 \tag{18}$$

can be solved for the case of the Coulomb potential $V(r) = -Z_{\alpha_1} Z_{\alpha_2} e^2/(4\pi\epsilon_0 r)$. The general solution is a linear combination of regular and irregular Coulomb wave functions. In the special case that $V(r) = 0$, such as for neutrons, equation (18), after a rearrangement in dimensionless form, is called the spherical Bessel equation. The solution consists of a linear combination of spherical Bessel functions of the first type $j_\ell(\rho)$, and of the second type $n_\ell(\rho)$ (or Neumann functions). Two linearly independent complex combinations of j_ℓ and n_ℓ are known as spherical Bessel functions of the third type (or Hankel functions) $h^+_\ell(\rho)$ and $h^-_\ell(\rho)$ [36, 37]. These are functions of the dimensionless parameter $\rho = kr$. Although $n_\ell(\rho) \to -\infty$ for $r \to 0$, this irregular solution should be included because we only need this solution in the external region $r > a_c$. The appropriate solution for a channel c is a linear combination of waves corresponding to incoming $I_c(r)$ and outgoing $O_c(r)$ waves for a free particle, $R(r) = R_\ell(r) = y_\ell I_\ell(r) + x_\ell O_\ell(r)$, with

$$I_c(r) = I_\ell(r) = -i\rho h^-_\ell(\rho) = -i\rho\Big(j_\ell(\rho) - i n_\ell(\rho)\Big) \tag{19}$$

and

$$O_c(r) = O_\ell(r) = -i\rho h^+_\ell(\rho) = i\rho\Big(j_\ell(\rho) + i n_\ell(\rho)\Big) \tag{20}$$

At large separation distances $r \to \infty$ the asymptotic forms of $I(r)$ and $O(r)$ correspond indeed to plain waves travelling in positive direction (outgoing waves) or negative direction (incoming waves). The functions $j_\ell(\rho)$ and $n_\ell(\rho)$ together with $O_\ell(\rho)$ are given in table 1. In figure 5 the function $j_\ell(\rho)$ is shown as a function of ρ and as a function of equivalent energy for a nucleus with mass $A = 238$.

1.3 The collision matrix U

The total wave function Ψ in the external region can be expressed as the superposition of all incoming and outgoing partial waves $\mathcal{I}_c$ and $\mathcal{O}_c$, with amplitudes y_c and x_c, and summed over all possible channels c.

$$\Psi = \sum_c y_c \mathcal{I}_c + \sum_{c'} x_{c'} \mathcal{O}'_c \tag{21}$$

The complete wave functions in the channel, $\mathcal{I}_c$ and $\mathcal{O}_c$, contain the radial parts I_c and O_c, but also the angular part of relative motion $Y^\ell_{m_\ell}$, as well as the internal

Table 1: The spherical Bessel functions and the incoming and outgoing waves from equations (19) and (20). Derived quantities are given in table 2.

ℓ	j_ℓ	n_ℓ	$O_\ell = I_\ell^*$
0	$\frac{\sin\rho}{\rho}$	$-\frac{\cos\rho}{\rho}$	$e^{i\rho}$
1	$\frac{\sin\rho}{\rho^2} - \frac{\cos\rho}{\rho}$	$-\frac{\cos\rho}{\rho^2} - \frac{\sin\rho}{\rho}$	$e^{i\rho}\left(\frac{1}{\rho} - i\right)$
ℓ	$(-1)^\ell \rho^\ell \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^\ell \frac{\sin\rho}{\rho}$	$-(-1)^\ell \rho^\ell \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^\ell \frac{\cos\rho}{\rho}$	

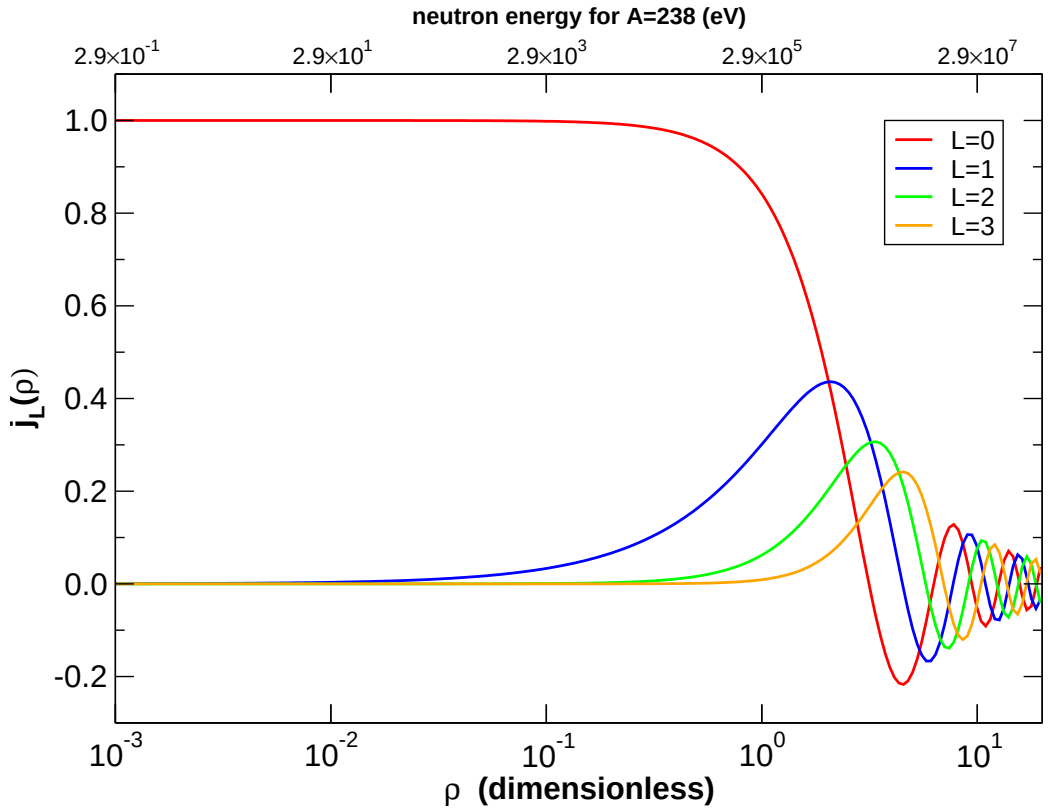

Figure 5: The Bessel function $j_\ell(\rho)$ for $\ell = 0, 1, 2, 3$ is shown as a function of ρ and as a function of equivalent energy for a nucleus with mass $A = 238$.

wave functions of the particles and the channel spin, combined in φ_c, and are written as

$$\mathcal{I}_c = I_c r^{-1} \varphi_c i^\ell Y^\ell_{m_\ell}(\theta,\phi)/\sqrt{v_c} \tag{22}$$

and

$$\mathcal{O}_c = O_c r^{-1} \varphi_c i^\ell Y^\ell_{m_\ell}(\theta,\phi)/\sqrt{v_c} \tag{23}$$

The factor $1/\sqrt{v_c}$ normalizes the waves to unit flux. The physical process of the reaction will result in a modification of the outgoing waves. In the reaction the coefficients x_c of the outgoing waves, depending on the details of the reaction which are observable in the cross section, have to be determined with respect to the coefficients of the incoming waves y_c. The collision matrix $U_{cc'}$ is now defined as the relation between the coefficients of the incoming and outgoing waves:

$$x_{c'} \equiv -\sum_c U_{c'c} y_c \tag{24}$$

All the physics of the reaction is contained in the elements of the collision matrix. The collision matrix has two important properties. From the conservation of probability flux in the reaction it follows that the collision matrix is unitary, which means that its complex conjugate equals its reciprocal, $\mathbf{U}^* = \mathbf{U}^{-1}$ or

$$\sum_c U^*_{cc'} U_{cc''} = \delta_{c'c''} \tag{25}$$

The second property follows from time reversal conservation and implies that the collision matrix is symmetric, $U_{cc'} = U_{c'c}$.

Finally we can express the total wave function of equation (21) in terms of the collision matrix:

$$\Psi = \sum_c y_c \left(\mathcal{I}_c - \sum_{c'} U_{cc'} \mathcal{O}_{c'} \right) \tag{26}$$

which is a linear combination of the wave functions for each channel c, consisting of an ingoing wave and the modified outgoing waves summed over all channels c'.

1.4 The relation between the cross sections and the collision matrix U

The relation between reaction cross section and wave functions, describing a probability, is based on the conservation of probability density. The probability density of an incident plain wave, which is the flux of particles $\mathbf{j}_\varphi$ is given by the quantum mechanical expression

$$\mathbf{j}_\varphi = \frac{\hbar}{2mi} \left(\psi^* \nabla \psi - \psi \nabla \psi^* \right) \tag{27}$$

The connection with the cross section is best illustrated by considering a flux of incident particles $j_{\rm inc}$, represented by a plain wave $\psi_{\rm inc}$ which can be expanded in a series of partial radial waves, scattering elastically at a point $r = 0$ because of an unknown physical process. The scattered wave, originating at $r = 0$ is a radial wave $\psi_{\rm sc}$ and far from the scattering center at a distance r in a solid angle element $d\Omega$ the current of scattered particles across the surface $r^2 d\Omega$ is $j_{\rm sc}$. The total wave $\psi = \psi_{\rm inc} + \psi_{\rm sc}$ is a solution of the Schrödinger equation for this system. The cross section of this reaction, which is a differential cross section, is defined as

$$d\sigma = \frac{j_{\rm sc}}{j_{\rm inc}} r^2 d\Omega \tag{28}$$

Integrating over $d\Omega$ gives the total scattering cross section. If elastic scattering were the only process to occur, the total current of ingoing particles equals that of the outgoing particles. Any reaction, defined as any other process than elastic scattering, means that there is a difference in the absolute values of the ingoing and outgoing current.

In the more general description of channels the total wave function is equation (26). Elastic scattering means here that the entrance and exit channel are the same. A change of channel in the outgoing wave is considered as a reaction. With a similar approach, including the expansion of the incoming plane wave into an infinite sum of partial waves ℓ, and using the full description of the channel wave functions, the angular differential cross section for the reaction $\alpha \rightarrow \alpha'$ has been worked out by Blatt and Biedenharn [38]. For zero Coulomb interaction the expression is

$$\frac{d\sigma}{d\Omega} = \frac{1}{2j+1} \lambda\!\!\!^{-2} \sum_{\ell=0}^{\infty} B_\ell(c, c') P_\ell(\cos\theta) \tag{29}$$

The coefficients $B_\ell(c, c')$ are rather complicated factors and contain the collision matrix elements $U_{cc'}$ and relations containing Clebsch-Gordan coefficients for the spin bookkeeping, eliminating most of the terms in the infinite sum over ℓ.

The cross section for an interaction from channel c to channel c' is then

$$\sigma_{cc'} = \pi \lambda\!\!\!^{-2}_c |\delta_{c'c} - U_{c'c}|^2 \tag{30}$$

If the interaction occurs without a change in the channel c then the process is called elastic scattering. The cross section is, putting $c' = c$

$$\sigma_{cc} = \pi \lambda\!\!\!^{-2}_c |1 - U_{cc}|^2 \tag{31}$$

and the cross section for a channel reaction, i.e. any interaction which is not elastic scattering, is obtained by summing (30) over all c' except c

$$\sigma_{cr} = \pi \lambda\!\!\!^{-2}_c (1 - |U_{cc}|^2) \tag{32}$$

and the total cross section is obtained by summing all channels c'

$$\sigma_{c,T} = \sigma_c = 2\pi\lambda\!\!\!^{-2}_c(1 - \mathrm{Re}\, U_{cc}) \tag{33}$$

In practise, channel to channel cross sections are not useful. One would like to have the cross sections of $\alpha \to \alpha'$ for the component of total angular momentum J. The total reaction cross section is obtained by integrating (29) over the full solid angle to obtain to total cross section for the component of total angular momentum J

$$\sigma_{\alpha\alpha'}(J) = \pi\lambda\!\!\!^{-2}_\alpha g(J) \sum_{j,j',\ell,\ell'} |\delta_{jj'\ell\ell'} - U_{j\ell,j'\ell'}|^2 \tag{34}$$

and the total cross section by summing over all α'

$$\sigma_{\alpha,T}(J) = 2\pi\lambda\!\!\!^{-2}_\alpha g(J) \sum_{j,\ell} (1 - \mathrm{Re}\, U_{j\ell,j\ell}) \tag{35}$$

1.5 The wave function in the internal region

The complete wave function Ψ can be described as the product of the function of relative motion and the channel-spin function, giving the internal states of the particles α_1 and α_2 and their combined spin. From the function of relative motion the radial part $R(r)$ is separated and the remaining part is combined with the channel-spin function to give the channel surface function φ_c

$$\Psi = \sum_c \varphi_c R_c(a_c)\,. \tag{36}$$

The surface functions φ_c have the property of orthonormality over the surface S_c given by $r = a_c$. This will be exploited to expand certain quantities in terms of surface functions. It follows immediately that

$$R_c(a_c) = \int \varphi_c^* \Psi dS_c\,. \tag{37}$$

The integration over a surface, instead of integrating over a volume, is particularly useful in deriving the R-matrix relation using Green's theorem, expressing a volume integral in a surface integral.

At the channel surface $r = a_c$ the radial wave function for the internal and external region should match. The value V_c and derivative D_c are defined with a normalization constant as

$$\begin{aligned} V_c &= \sqrt{\frac{\hbar^2}{2m_c a_c}}\, u_c(a_c) \\ &= \sqrt{\frac{\hbar^2}{2m_c a_c}} \int \varphi_c^* \Psi dS_c \end{aligned} \tag{38}$$

and

$$\begin{aligned} D_c &= \sqrt{\frac{\hbar^2}{2m_c a_c}} a_c \left(\frac{du_c}{dr}\right)_{r=a_c} \\ &= \sqrt{\frac{\hbar^2}{2m_c a_c}} \int \varphi_c^* \nabla_{\mathrm{n}} (r\Psi) dS_c \\ &= V_c + \sqrt{\frac{\hbar^2}{2m_c a_c}} a_c \int \varphi_c^* dS_c \end{aligned} \tag{39}$$

In the internal region the wave function cannot be calculated readily by solving the Schrödinger equation since the nuclear potential is in general very complicated and the nucleus has many interacting nucleons. But the wave function can be expressed as an expansion in eigenfunctions X_λ and eigenvalues E_λ

$$\Psi = \sum_\lambda A_\lambda X_\lambda \tag{40}$$

and the coefficients A_λ can be expressed as

$$A_\lambda = \int X_\lambda^* \Psi d\tau \tag{41}$$

where the integration goes over the volume $d\tau$ of the internal region given by $r < a_c$.

The values and derivatives on the surface $r = a_c$ are defined, analog to equation (38) and (39), as

$$\gamma_{\lambda c} = \sqrt{\frac{\hbar^2}{2m_c a_c}} \int \varphi_c^* X_\lambda dS_c \tag{42}$$

and

$$\delta_{\lambda c} = \gamma_{\lambda c} + \sqrt{\frac{\hbar^2}{2m_c a_c}} a_c \int \varphi_c^* \nabla_{\mathrm{n}} (X_\lambda) dS_c \,. \tag{43}$$

The boundary conditions to be satisfied on the channel surface are taken identical for all λ

$$B_c = \delta_{\lambda c} / \gamma_{\lambda c} \,. \tag{44}$$

Applying Green's theorem to equation (41) gives

$$\begin{aligned} A_\lambda &= \int X_\lambda^* \Psi d\tau \\ &= (E_\lambda - E)^{-1} \frac{\hbar^2}{2m_c} \int \left(X_\lambda^* \nabla_{\mathrm{n}}(\Psi) - \Psi \nabla_{\mathrm{n}}(X_\lambda^*)\right) dS_c \\ &= (E_\lambda - E)^{-1} \sum_c (D_c - B_c V_c) \gamma_{\lambda c} \end{aligned} \tag{45}$$

using equations (38), (39), (42), (43) and (44). The expression (40) for the wave-function can now be written as

$$\Psi = \sum_c \left[\sum_\lambda \frac{X_\lambda \gamma_{\lambda c}}{E_\lambda - E} \right] (D_c - B_c V_c) \,. \tag{46}$$

By multiplying each side of equation (46) by $\varphi_{c'}$, integrating over the surface $r = a_c$ and using equation (42) one obtains

$$V_{c'} = \sum_c R_{cc'} (D_c - B_c V_c) \tag{47}$$

with

$$R_{cc'} = \sum_\lambda \frac{\gamma_{\lambda c} \gamma_{\lambda c'}}{E_\lambda - E} \,. \tag{48}$$

The quantity $R_{cc'}$ is the R-matrix and contains the properties E_λ and $\gamma_{\lambda c}$ of the eigenstates λ. The boundary constant B_c can be chosen freely.

1.6 The relation between the R-matrix and the collision matrix U

The values and derivatives of the internal wave function are given by the R-matrix relation equation (47). The external wave function is given by equation (26) and is known except for the boundary conditions. The boundary condition is that both the internal and external wave functions have the same value and radial derivative at $r = a_c$ in order to have a smooth transition. By matching these conditions and after considerable rearrangements, the collision matrix $U_{cc'}$ can be given explicitly as a function of the R-matrix in matrix notation by

$$\mathbf{U} = \mathbf{\Omega P}^{1/2} [\mathbf{1} - \mathbf{R}(\mathbf{L} - \mathbf{B})]^{-1} [\mathbf{1} - \mathbf{R}(\mathbf{L}^* - \mathbf{B})] \mathbf{P}^{-1/2} \mathbf{\Omega} \,. \tag{49}$$

The introduced complex matrix $\mathbf{L}$ is given by

$$L_c = S_c + iP_c = \left(\frac{\rho}{O_c} \frac{dO_c}{d\rho} \right)_{r=a_c} \tag{50}$$

where real matrices S_c is called the shift factor and P_c the penetrability factor. The matrix Ω_c is

$$\Omega_c = \left(\frac{I_c}{O_c} \right)_{r=a_c} \tag{51}$$

which can be reduced for neutral particles, using equations (19) and (20), to

$$\Omega_c = \exp(-i\phi_c) \tag{52}$$

from which ϕ_c follows

$$\phi_c = \arg O_c(a_c) = \arctan \left(\frac{\mathrm{Im}\, O_c}{\mathrm{Re}\, O_c} \right) = \arctan \left(-\frac{j_\ell(\rho)}{n_\ell(\rho)} \right) \tag{53}$$

All matrices in equation (49) are diagonal matrices except **U** and **R**. A table of P_ℓ, S_ℓ and ϕ_ℓ is given below. They are directly related to the solution of the Schrödinger equation in the external region, which are the spherical Bessel and Neumann functions $j_\ell(\rho)$ and $n_\ell(\rho)$ for neutral particles, and can be derived from the quantities listed in table 1.

If the boundary conditions B_c, defined by equation (44), are real, then the $\delta_{\lambda c}$ and the $\gamma_{\lambda c}$ are real and hence **R** is real. In addition **R** is symmetrical. A common choice is to take

$$B_c = S_c \tag{54}$$

which eliminates the shift factor for s-waves, but introduces an energy dependence. The choice $B_c = -\ell$ has also been proposed [24]. At low energy this is equivalent as can be seen in figure 6, where P_ℓ, S_ℓ and ϕ_ℓ are plotted as a function of ρ and as a function of equivalent energy for a nucleus with mass $A = 238$.

Table 2: The penetrability P_ℓ, the level shift S_ℓ and the hard-sphere phase shift ϕ_ℓ for reaction channels without Coulomb interaction, as a function of $\rho = ka_c$. These parameters are derived from the quantities in table 1.

ℓ	P_ℓ	S_ℓ	ϕ_ℓ
0	ρ	0	ρ
1	$\rho^3/(1+\rho^2)$	$-1/(1+\rho^2)$	$\rho - \arctan\rho$
ℓ	$\frac{\rho^2 P_{\ell-1}}{(\ell-S_{\ell-1})^2+P_{\ell-1}^2}$	$\frac{\rho^2(\ell-S_{\ell-1})}{(\ell-S_{\ell-1})^2+P_{\ell-1}^2} - \ell$	$\phi_{\ell-1} - \arctan\frac{P_{\ell-1}}{\ell-S_{\ell-1}}$

So equation (49) defines the collision matrix in terms of the parameters of the R-matrix, $\gamma_{\lambda c}$ and E_λ, representing the physical process of the reaction, and the quantities P_c, S_c, ϕ_c, describing the known incoming and outgoing waves I_c and O_c, outside a sphere with radius a_c. The values B_c determine the boundary conditions at the matching point of the internal and external region, and are free to be chosen. The unknowns of the R-matrix, $\gamma_{\lambda c}$ and E_λ, need to be determined in order to know the U-matrix and subsequently the cross sections.

1.7 Approximations of the R-matrix

Several approximations of the R-matrix have been developed in the past in order to overcome the complications of inverting the matrix

$$[\mathbf{1} - \mathbf{R}(\mathbf{L} - \mathbf{B})]^{-1}$$

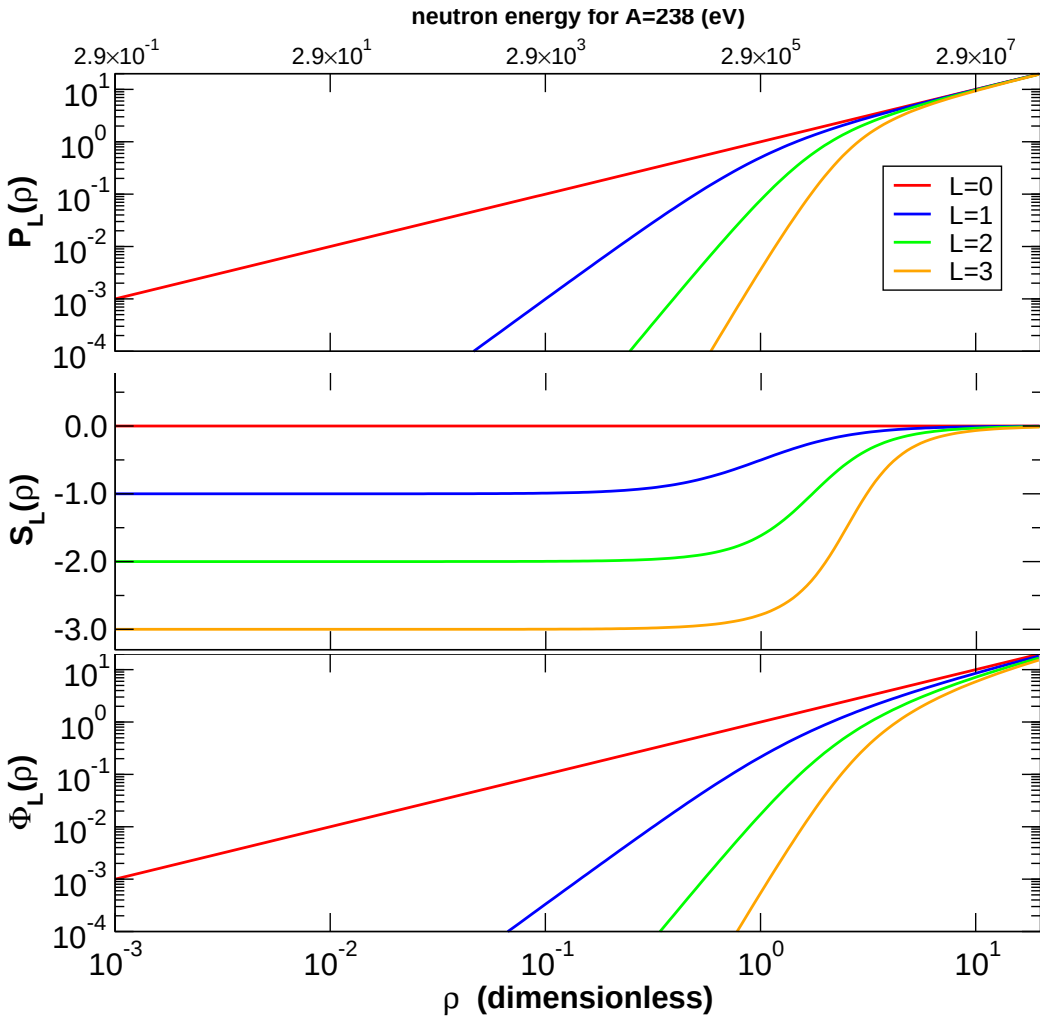

Figure 6: The functions $P_\ell(\rho)$, $S_\ell(\rho)$ and $\phi_\ell(\rho)$ for $\ell = 0, 1, 2, 3$ shown as a function of ρ and as a function of equivalent energy for a nucleus with mass $A = 238$.

appearing in equation (49). Except in the case where only 1 or 2 channels are involved, the inversion is in general impossible without additional assumptions. The problem can be put in terms of the inversion of a level matrix $\mathbf{A}$ of which the elements refer to the properties of the levels λ of the system. The problem of inverting a matrix concerning all channels is now put in a problem of inverting a matrix concerning levels.

The level matrix $A_{\lambda\mu}$ is introduced by putting the following form

$$\left([\mathbf{1} - \mathbf{R}(\mathbf{L} - \mathbf{B})]^{-1} \right)_{cc'} = \delta_{cc'} + \sum_{\lambda\mu} \gamma_{\lambda c} \gamma_{\mu c'} (L_{c'} - B_{c'}) A_{\lambda\mu} \tag{55}$$

from which the elements of the inverse of $\mathbf{A}$ are

$$\begin{aligned}\left(\mathbf{A}^{-1}\right)_{\lambda\mu} &= (E_\lambda - E)\delta_{\lambda\mu} - \sum_c \gamma_{\lambda c}\gamma_{\mu c}(L_c - B_c) \\ &= (E_\lambda - E)\delta_{\lambda\mu} - \Delta_{\lambda\mu} - \frac{1}{2}i\Gamma_{\lambda\mu}\end{aligned} \tag{56}$$

with the quantities $\Delta_{\lambda\mu}$ and $\Gamma_{\lambda\mu}$ defined by

$$\Delta_{\lambda\mu} = \sum_c (S_c - B_c)\gamma_{\lambda c}\gamma_{\mu c} \tag{57}$$

and

$$\Gamma_{\lambda\mu} = 2\sum_c P_c \gamma_{\lambda c}\gamma_{\mu c} \tag{58}$$

Now the collision matrix from equation (49) can be expressed in terms of $\mathbf{A}$

$$U_{cc'} = \Omega_c \Omega_{c'} \left(\delta_{cc'} + 2i\sqrt{P_c P_{c'}} \sum_{\lambda\mu} A_{\lambda\mu}\gamma_{\lambda c}\gamma_{\mu c'} \right) \tag{59}$$

Additional approximations have been formulated in order to simplify this expression. The most illustrative is the Breit and Wigner Single Level (SLBW) approximation where only one level is considered. It can be extended to several, independent levels, which is the Breit and Wigner Multi Level (MLBW) approximation. The formalism of Reich and Moore [39] neglects only the off-diagonal contributions of the photon channels, which is an accurate approximation for medium and heavy nuclei. It takes into account the interference between levels and reduces to the BWSL approximation in the limit of a single level. These three formalisms will be described in some more detail. Other formalisms exist of which we mention here the formalisms of Kapur and Peierls [40], Wigner and Eisenbud [22], Adler and Adler [29], Hwang [41] and more recently Luk'yanov and Yaneva [34].

1.8 The Breit-Wigner Single Level approximation

The expression equation (56) can be simplified if only a single level is present. In that case the matrix contains only a single element. Therefore

$$\left(\mathbf{A}^{-1}\right)_{\lambda\mu} = A^{-1} = E_\lambda - E + \Delta_\lambda - i\Gamma_\lambda/2 \tag{60}$$

with

$$\Delta_\lambda = \Delta_{\lambda\lambda} = -\sum_c (S_c - B_c)\gamma_{\lambda c}^2 \tag{61}$$

and

$$\Gamma_\lambda = \Gamma_{\lambda\lambda} = \sum_c \Gamma_{\lambda c} = \sum_c 2P_c\gamma_{\lambda c}^2 \tag{62}$$

Substituting these expressions in equation (59) gives the collision matrix

$$U_{cc'} = e^{-i(\phi_c+\phi_{c'})}\left(\delta_{cc'} + \frac{i\sqrt{\Gamma_{\lambda c}\Gamma_{\mu c'}}}{E_\lambda + \Delta_\lambda - E - i\Gamma_\lambda/2}\right) \tag{63}$$

From the collision matrix the cross sections can be calculated. For the total cross section this results in

$$\sigma_c = \pi\lambda\!\!\!^{-2}_c g_c\left(4\sin^2\phi_c + \frac{\Gamma_\lambda\Gamma_{\lambda c}\cos 2\phi_c + 2(E - E_\lambda - \Delta_\lambda)\Gamma_{\lambda c}\sin 2\phi_c}{(E - E_\lambda - \Delta_\lambda)^2 + \Gamma_\lambda^2/4}\right) \tag{64}$$

The first part of the total cross section is the potential scattering or hard sphere scattering cross section $\sigma_p = 4\pi\lambda\!\!\!^{-2}_c g_c \sin^2\phi_c$. It is associated with the elastic scattering of the incoming neutron from the potential of the nucleus without forming a compound state. The term with the factor $\sin 2\phi_c$ is the interference of the potential scattering and the resonant elastic scattering through formation of a compound nucleus. Finally the term with $\cos 2\phi_c$ describes the resonance cross sections of the channels.

In a more practical case we can see what the cross sections becomes for a neutron entrance channel $c = n$. We assume that the only open channels are elastic scattering and neutron capture, $\Gamma_\lambda = \Gamma = \Gamma_n + \Gamma_\gamma$.

A series expansion of the trigoniometric factors gives for $\ell = 0$ at low energy in good approximation $\sin\phi_c = \rho = ka_c$ and $\sin\phi_c = 0$ for $\ell > 0$. The cosine term can be approximated by $\cos\phi_c = 1$ for all ℓ.

In the same way, the reaction cross section is

$$\sigma_{cc'} = \pi\lambda\!\!\!^{-2}_c g_c \frac{\Gamma_{\lambda c}\Gamma_{\lambda c'}}{(E - E_\lambda - \Delta_\lambda)^2 + \Gamma_\lambda^2/4} \tag{65}$$

and the shift Δ_λ results from the boundary condition.

1.9 The Breit-Wigner Multi Level approximation

Several resonances can be taken into account as a sum of Breit and Wigner single level cross sections. This is the most simple treatment of cross sections of many resonances. It neglects any possible interference between channels and levels (resonances).

The Breit and Wigner multi level (BWML) approach uses a sum over the levels in the collision matrix. In the inverse of the level matrix $\mathbf{A}$ all off-diagonal elements $A_\lambda^{-1}\mu$ are neglected, which means neglecting all interference terms between channels, but not between levels.

$$\left(\mathbf{A}^{-1}\right)_{\lambda\mu} = (E_\lambda - E + \Delta_\lambda - i\Gamma_\lambda/2)\delta_{\lambda\mu} \tag{66}$$

$$U_{cc'} = e^{-i(\phi_c+\phi_{c'})}\left(\delta_{cc'} + \sum_\lambda \frac{i\sqrt{\Gamma_{\lambda c}\Gamma_{\mu c'}}}{E_\lambda + \Delta_\lambda - E - i\Gamma_\lambda/2}\right) \tag{67}$$

1.10 The Reich-Moore approximation

In the approximation of Reich and Moore [39] it is assumed that the amplitudes $\gamma_{\lambda c}$ are uncorrelated and have a Gaussian distribution with zero mean. This is a consequence of the chaotic behaviour of the compound nucleus, except for the very light nuclei. This is known as the Gaussian Orthogonal Ensemble [1, 2, 5].

In medium and heavy nuclei, the number of photon channels is very large. And since the amplitudes are supposed to have a random distribution with zero mean, the expectation value of the product of two amplitudes is zero for $\lambda \neq \mu$, i.e. $< \gamma_{\lambda c}\gamma_{\mu c} >= \gamma_{\lambda c}^2\delta_{\lambda\mu}$. Summing over the photon channels gives

$$\sum_{c\in\text{photon}} \gamma_{\lambda c}\gamma_{\mu c} = \sum_{c\in\text{photon}} \gamma_{\lambda c}^2\delta_{\lambda\mu} = \Gamma_{\lambda\gamma}\delta_{\lambda\mu} \tag{68}$$

Therefore the general expression for $\mathbf{A}^{-1}$, equation (56), can be simplified for the photon channels and becomes

$$\begin{aligned}\left(\mathbf{A}^{-1}\right)_{\lambda\mu} &= (E_\lambda - E)\delta_{\lambda\mu} - \sum_{c\in\text{photon}} \gamma_{\lambda c}\gamma_{\mu c}(L_c - B_c) - \sum_{c\notin\text{photon}} \gamma_{\lambda c}\gamma_{\mu c}(L_c - B_c) \\ &= (E_\lambda - E)\delta_{\lambda\mu} - \Gamma_{\lambda\gamma}(L_c - B_c)\delta_{\lambda\mu} - \sum_{c\notin\text{photon}} \gamma_{\lambda c}\gamma_{\mu c}(L_c - B_c) \\ &= (E_\lambda - E + \Delta_\lambda - i\Gamma_{\lambda\gamma}/2)\delta_{\lambda\mu} - \sum_{c\notin\text{photon}} \gamma_{\lambda c}\gamma_{\mu c}(L_c - B_c)\end{aligned} \tag{69}$$

Comparing this to equation (56), the approximation may be written as a reduced R-matrix in the sense that the photon channels are excluded and the eigenvalue E_λ is replaced by $E_\lambda - i\Gamma_{\lambda\gamma}/2$. This Reich-Moore R-matrix is

$$R_{cc'} = \sum_\lambda \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_\lambda - E - i\Gamma_{\lambda\gamma}/2} \qquad c \notin \text{photon} \tag{70}$$

The number of energy levels, which may be over hundreds of thousands in heavy nuclei, determines the number of possible photon decay channels. Excluding them reduces largely the number of channels and therefore the matrix inversion needed in the relation between the R-matrix and the cross sections. In the often occurring case at low energy that only the elastic scattering and neutron capture channels are open, the number of channels in the R-matrix is one, namely that of the neutron channel, the photon channels being excluded explicitly. The total radiation width is present however in the denominator of equation (70). The R-matrix becomes in this case an R-function of which the inversion is trivial.

Including other channels, like one or two fission channels, keeps the number of channels low and makes the inversion still feasible. This approximation of the general R-matrix is the most accurate one used.

2 Average cross sections

At higher energies the widths of the resonances overlap and the cross sections appear smooth and with a slow variation with energy. The total and scattering cross sections without sharply separated or observed resonances can be adequately described by representing the particle-nucleus interaction by a complex potential. This optical potential, so called because mathematically analogous to the scattering and absorption of light in a medium (cloudy crystal ball), results in the partial scattering or absortion of the beam. The solution of the Schrödinger equation, usually numerically, with a given potential gives the wave functions from which the cross sections can be obtained [42]. Much progress has been made since in the theoretical development and parametrization of a suitable optical model potentials, see for example refs. [19, 43–47].

By making averages over resonances, the energy averaged collision matrix $\overline{U_{cc}}$ can be related to the energy-averaged cross sections $\overline{\sigma}$. The development of a given shape of the optical model potential results in a value for $\overline{U_{cc}}$. From the usual R-matrix expressions we can formulate a number of cross sections as follows. By analogy to equation (31) the average scattering cross section $\overline{\sigma_{cc}}$ can be written as

$$\overline{\sigma_{cc}} = \pi\lambda_c^2 g_c \overline{|1 - U_{cc}|^2} \tag{71}$$

which can be split up into an average shape elastic scattering cross section

$$\overline{\sigma_{cc}^{\mathrm{se}}} = \pi\lambda_c^2 g_c |1 - \overline{U_{cc}}|^2 \tag{72}$$

associated with potential scattering, and an average compound elastic scattering cross section due to resonance scattering

$$\overline{\sigma_{cc}^{\mathrm{ce}}} = \pi\lambda_c^2 g_c \left(\overline{|U_{cc}|^2} - |\overline{U_{cc}}|^2 \right) \tag{73}$$

and after equation (32) the average reaction cross section $\overline{\sigma_{cr}}$, corresponding to all non-elastic partial cross sections, as

$$\overline{\sigma_{cr}} = \pi\lambda_c^2 g_c (1 - \overline{|U_{cc}|^2}) \tag{74}$$

and following equation (33) the average total cross section $\overline{\sigma_c, T}$ can be written as

$$\overline{\sigma_{c,T}} = 2\pi\lambda_c^2 g_c (1 - \mathrm{Re}\,\overline{U_{cc}})\,. \tag{75}$$

The sum of the average compound elastic scattering cross section $\overline{\sigma_{cc}^{\mathrm{ce}}}$ and the average reaction cross section $\overline{\sigma_{cr}}$ can be considered as the cross section for the formation of the compound nucleus $\overline{\sigma_c}$, and can be written as

$$\begin{aligned}\overline{\sigma_c} = \overline{\sigma_{cc}^{\mathrm{ce}}} + \overline{\sigma_{cr}} &= \pi\lambda_c^2 g_c \left(\overline{|U_{cc}|^2} - |\overline{U_{cc}}|^2 + 1 - \overline{|U_{cc}|^2} \right) \\ &= \pi\lambda_c^2 g_c (1 - |\overline{U_{cc}}|^2)\end{aligned} \tag{76}$$

Then the sum of this compound nucleus formation cross section $\overline{\sigma_c}$ and the average shape elastic scattering cross section $\overline{\sigma_{cc}^{\mathrm{se}}}$ equals the total cross section $\overline{\sigma_{c,T}}$, which can be checked by

$$\begin{aligned}\overline{\sigma_c} + \overline{\sigma_{cc}^{\mathrm{se}}} &= \pi\lambda_c^2 g_c \left(1 - |\overline{U_{cc}}|^2 + |1 - \overline{U_{cc}}|^2\right) \\ = \pi\lambda_c^2 g_c \left(1 - |\overline{U_{cc}}|^2 + 1 - 2\,\mathrm{Re}\,\overline{U_{cc}} + |\overline{U_{cc}}|^2\right) &= \overline{\sigma_{c,T}}\end{aligned} \tag{77}$$

From the above expressions, only the total, shape elastic, and compound nucleus formation cross sections $\overline{\sigma_{c,T}}$ $\overline{\sigma_{cc}^{\mathrm{se}}}$, and $\overline{\sigma_c}$ contain the elements $\overline{U_{cc}}$, calculated by optical model, without other terms like $\overline{|U_{cc}|^2}$ which cannot be extracted from optical model calculations. For a direct comparison with experimental data, only the calculated average total cross section (equation (75)) can be used in a general way. The shape elastic scattering cross section cannot be distinguished from the compound elastic scattering. The calculated compound nucleus formation cross section (equation (76)) is also not directly observable, but can be used in combination with measured decay channels, like in the surrogate measurements.

Finally the average cross section for a single reaction $\overline{\sigma_{cc'}}$ is

$$\overline{\sigma_{cc'}} = \pi\lambda_c^2 g_c \overline{|\delta_{cc'} - U_{cc'}|^2} \tag{78}$$

which contains the nearly impossible averaging over $|U_{cc'}|^2$.

When we introduce the transmission coefficient

$$T_c = 1 - |U_{cc}|^2 \tag{79}$$

the compound nucleus formation cross section (unaveraged) can be written as

$$\sigma_c = \pi\lambda_c^2 g_c T_c \tag{80}$$

Using the usual concepts in nuclear reaction theory (reciprocity, time-reversal invariance), the probability of decay through channel c' as $T_{c'}/\Sigma T_i$ the cross section for the reaction $c \to c'$ is then

$$\sigma_{cc'} = \pi\lambda_c^2 g_c T_c \frac{T_{c'}}{\Sigma T_i} \tag{81}$$

where the sum runs over all possible channels. Averaging over a small energy interval with many resonances, taking into account shape elasting in addition to compound reactions and redefining T_c as

$$T_c = 1 - |\overline{U_{cc}}|^2 \tag{82}$$

results in the Hauser-Feshbach formula (see also [24, 48–55] for more details)

$$\overline{\sigma_{cc'}} = \overline{\sigma_{cc}^{\mathrm{se}}}\delta_{cc'} + \pi\lambda\!\!\!^{-2}_{c} g_c \frac{T_c T_{c'}}{\Sigma T_i} W_{cc'} \tag{83}$$

where the factor $W_{cc'}$ is factor which includes elastic enhancement and a correction for width fluctuations, which can be written as (see for example ref. [53])

$$W_{cc'} = \overline{\left(\frac{\Gamma_c \Gamma_{c'}}{\Gamma}\right)} \frac{\overline{\Gamma}}{\overline{\Gamma_c}\,\overline{\Gamma_{c'}}} \tag{84}$$

The width fluctuations can be calculated most accurately using the GOE triple integral [56, 57], but also with simpler approximations.

The transmission coefficients for particle channels are given by equation (82). Two other channels exist which are the photon and fission channels. Their transmission coefficients, related to the average widths and level spacing, are defined as

$$T_\gamma = 2\pi \frac{\overline{\Gamma_\gamma}}{D} \tag{85}$$

and

$$T_f = 2\pi \frac{\overline{\Gamma_f}}{D} \tag{86}$$

Dedicated modelizations on photon strength functions, level densities and fission models, are used for the photon and fission transmission coefficients, but are beyond the scope of this overview. Good starting points for further reading are the user guides of specialized computer codes like EMPIRE [58], TALYS [59], and others.

Concluding remarks

The importance of neutron induced reaction data is evident in a wide variety of research fields, ranging from stellar nucleosynthesis and nuclear structure to applications of nuclear technology. The present overview has sketched out an introduction of the reaction description using the *R*-matrix formalism. Many details were intentionally omitted but the provided references should form a good starting point for the interested reader.

References

[1] J. E. Lynn. *The Theory of Neutron Resonance Reactions*. Clarendon Press, Oxford, 1968.

[2] M. L. Mehta. In: *Nucl. Phys.* 18 (1960), p. 395.

[3] R. U. Haq, A. Pandey, and O. Bohigas. "Fluctuations Properties of Nuclear Energy Levels: Do Theory and Experiment Agree?" In: *Phys. Rev. Lett.* 48.6 (1982), pp. 1086–1089.
[4] O. Bohigas, M. J. Giannoni, and C. Schmit. "Characterization of chaotic quantum spectra and universality of level fluctuation laws". In: *Phys. Rev. Lett.* 52 (1984), pp. 1–4.
[5] M. L. Mehta. *Random matrices*. Academic Press. 1991.
[6] C. E. Porter and R. G. Thomas. "Fluctuations of Nuclear Reaction Widths". In: *Phys. Rev.* 104.2 (1956), pp. 483–491.
[7] C. Wagemans. *The Nuclear Fission Process*. CRC, 1991.
[8] A. Gilbert and A. G. W. Cameron. In: *Can. J. Phys.* 43.3 (1965), p. 1446.
[9] S. F. Mughabghab, M. Divadeenam, and N. E. Holden. *Neutron cross sections: Neutron resonance parameters and thermal cross sections. Z=1-60*. Academic Press, 1981.
[10] S. F. Mughabghab, M. Divadeenam, and N. E. Holden. *Neutron cross sections: Neutron resonance parameters and thermal cross sections. Z=61-100*. Academic Press, 1984.
[11] S. F. Mughabghab. *Atlas of Neutron Resonances*. Elsevier Science, 2006.
[12] S. I. Sukhoruchkin, Z. N. Soroko, and V. V. Deriglazov. *Low Energy Neutron Physics, Volume I/16B, Tables of Neutron Resonance Parameters*. Springer, Landolt-Börnstein, 1998.
[13] S. I. Sukhoruchkin and Z. N. Soroko. *Elementary Particles, Nuclei and Atoms, Subvolume 26A. Supplement to I/24, Neutron Resonance Parameters*. Springer, Landolt-Börnstein, 2015.
[14] *BROND*. Tech. rep. Institute of Physics and Power Engineering,Obninsk, Russian Federation.
[15] M. B. Chadwick et al. "ENDF/B-VII.0: Next generation evaluated nuclear data library for nuclear science and technology. ENDF data can be accessed at the National Nuclear Data Center at Brookhaven National Laboratory [www.nndc.bnl.gov]". In: *Nuclear Data Sheets* 107.12 (2006), pp. 2931–3059.
[16] A. Koning et al. *The JEFF-3.1 Nuclear Data Libaray, JEFF Report 21*. Tech. rep. JEFF data can be accessed at the OECD Nuclear Energy Agency, 2006.
[17] K. Shibata et al. "Japanese evaluated nuclear data library version 3 revision-3: JENDL-3.3". In: *J. Nucl. Sci. Technol.* 39.11 (2002), pp. 1125–1136.
[18] *CENDL*. Tech. rep. Chinese Nuclear Data Center, Institute of Atomic Energy, P.O. Box 275(41) Beijing P.R.China.
[19] E. Bauge, J. P. Delaroche, and M. Giro. "Lane-consistent, semimicroscopic nucleon-nucleus optical model". In: *Phys. Rev. C* 63 (2001), p. 024607.
[20] G. L. Payne and L. Schlessinger. "Properties of the K Matrix in Nuclear-Reaction Theory". In: *Phys. Rev. C* 2.5 (1970), pp. 1648–1653.
[21] R. Shyam and O. Scholten. "Photoproduction of eta mesons within a coupled-channels [sans-serif K]-matrix approach". In: *Phys. Rev. C* 78.6 (2008), p. 065201.
[22] E. P. Wigner and L. Eisenbud. "Higher Angular Momenta and Long Range Interaction in Resonance Reactions". In: *Phys. Rev.* 72.1 (1947), pp. 29–41.

[23] A. M. Lane and R. G. Thomas. "R-Matrix Theory of Nuclear Reactions". In: *Rev. Mod. Phys.* 30.2 (1958), pp. 257–353.
[24] F. Fröhner. *Evaluation and Analysis of Nuclear Resonance Data*. Tech. rep. JEFF Report 18. OECD/NEA, 2000.
[25] J. Humblet and L. Rosenfeld. "Theory of nuclear reactions: I. Resonant states and collision matrix". In: *Nucl. Phys.* 26.4 (1961), pp. 529–578.
[26] E. Vogt. "Theory of Low Energy Nuclear Reactions". In: *Rev. Mod. Phys.* 34.4 (1962), pp. 723–747.
[27] F. Schmittroth and W. Tobocman. "Comparison of the *R*-Matrix Nuclear Reaction Theories". In: *Phys. Rev. C* 3 (1971), pp. 1010–1019.
[28] A. Foderaro. *The Elements of Neutoron Interaction Theory*. MIT Press, 1971.
[29] D. B. Adler and F. T. Adler. "Uniqueness of *R*-Matrix Parameters in the Analysis of Low-Energy Neutron Cross Sections of Fissile Nuclei". In: *Phys. Rev. C* 6 (1972), pp. 986–1001.
[30] C. Chandler and W. Tobocman. "*R*-matrix method for nuclear reaction theory". In: *Phys. Rev. C* 19 (1979), pp. 1660–1666.
[31] T. A. Brody, J. Flores, J. B. French, et al. "Random-matrix physics: spectrum and strength fluctuations". In: *Rev. Mod. Phys.* 53 (1981), pp. 385–479.
[32] J Humblet. "*K*-matrix analysis of resonance nuclear reactions". In: *Phys. Rev. C* 42.4 (1990), pp. 1582–1591.
[33] H. Feshbach. *Theoretical Nuclear Physics; Nuclear Reactions*. John Wiley & Sons, 1991.
[34] A. A. Luk'yanov and N. B. Yaneva. "Multilevel parametrization of resonance neutron cross sections". In: *Phys. Part. Nucl.* 28 (1997), pp. 331–347.
[35] C. R. Brune. "Alternative parametrization of *R*-matrix theory". In: *Phys. Rev. C* 66.044611 (2002).
[36] M. Abramowitz. *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Table*. Dover Publications, New York, 1965.
[37] Zwillinger D. *CRC Standard Mathematical Tables and Formulae*. CRC Press, 2003.
[38] J. M. Blatt and L. C. Biedenharn. "The Angular Distribution of Scattering and Reaction Cross Sections". In: *Rev. Mod. Phys.* 24.4 (1952), pp. 258–272.
[39] C. W. Reich and M. S. Moore. "Multilevel Formula for the Fission Process". In: *Phys. Rev.* 111.3 (1958), pp. 929–933.
[40] P. L. Kapur and R. E. Peierls. In: *Proc. Roy. Soc.* A166 (1938), p. 277.
[41] R. N. Hwang. In: *Nucl. Sci. Eng.* 52 (1973), p. 157.
[42] S. Fernbach, R. Serber, and T. B. Taylor. "The Scattering Of High Energy Neutrons By Nuclei". In: *Phys. Rev.* 75.9 (1949), pp. 1352–1355.
[43] H. S. Camarda, F. S. Dietrich, and T. W. Phillips. "Microscopic Optical-Model Calculations Of Neutron Total Cross-Sections and Cross-Section Differences". In: *Phys. Rev. C* 39.5 (1989), pp. 1725–1729.
[44] H. Leeb and S. Wilmsen. "Violation Of Pseudospin Symmetry In Nucleon-Nucleus Scattering: Exact Relations". In: *Phys. Rev. C* 62.2 (2000).

[45] F. S. Dietrich, J. D. Anderson, R. W. Bauer, et al. “Importance Of Isovector Effects In Reproducing Neutron Total Cross Section Differences In The W Isotopes”. In: *Phys. Rev. C* 67.4 (2003).
[46] R. Capote, E. S. Soukhovitskii, J. M. Quesada, et al. “Is a global coupled-channel dispersive optical model potential for actinides feasible?” In: *Phys. Rev. C* 72.6 (2005).
[47] J. M. Quesada, R. Capote, E. S. Soukhovitskii, et al. “Approximate Lane consistency of the dispersive coupled-channels potential for actinides”. In: *Phys. Rev. C* 76.5 (2007).
[48] W. Hauser and H. Feshbach. “The Inelastic Scattering Of Neutrons”. In: *Phys. Rev.* 87.2 (1952), pp. 366–373.
[49] H. Feshbach, C. E. Porter, and V. F. Weisskopf. “Model For Nuclear Reactions With Neutrons”. In: *Phys. Rev.* 96.2 (1954), pp. 448–464.
[50] P. E. Hodgson. *Nuclear Reactions and Nuclear Structure*. Clarendon Press, Oxford, 1971.
[51] P. A. Moldauer. “Why Hauser-Feshbach Formula Works”. In: *Phys. Rev. C* 11.2 (1975), pp. 426–436.
[52] P. A. Moldauer. “Direct Reaction Effects On Compound Cross-Sections”. In: *Phys. Rev. C* 12.3 (1975), pp. 744–756.
[53] P. A. Moldauer. “Evaluation Of Fluctuation Enhancement Factor”. In: *Phys. Rev. C* 14.2 (1976), pp. 764–766.
[54] P. A. Moldauer. “Statistics and The Average Cross-Section”. In: *Nucl. Phys. A* 344.2 (1980), pp. 185–195.
[55] I. Sirakov, R. Capote, F. Gunsing, et al. “An ENDF-6 compatible evaluation for neutron induced reactions of Th-232 in the unresolved resonance region”. In: *Ann. Nucl. Energy* 35.7 (2008), pp. 1223–1231.
[56] J. J. M. Verbaarschot, H. A. Weidenmuller, and M. R. Zirnbauer. “Grassmann Integration In Stochastic Quantum Physics – The Case Of Compound Nucleus Scattering”. In: *Phys. Rep. - Rev. Sect. Phys. Lett.* 129.6 (1985), pp. 367–438.
[57] J. J. M. Verbaarschot. “Investigation of the formula for the average of two S-matrix elements in compound nucleus reactions”. In: *Ann. Phys.* 168.2 (1986), pp. 368–386.
[58] M. Herman, R. Capote, B. V. Carlson, et al. “EMPIRE: Nuclear reaction model code system for data evaluation”. In: *Nucl. Data Sheets* 108.12 (2007), pp. 2655–2715.
[59] A. J. Koning, S. Hilaire, and M. Duijvestijn. *TALYS A nuclear reaction program*. Tech. rep. 2007.