RADCAP: a potential model tool for direct capture reactions

C.A. Bertulani

National Superconducting Cyclotron Laboratory,

Michigan State University, East Lansing, MI 48824, USA[*]

(Dated: July 24, 2003)

Abstract

A computer program is presented aiming at the calculation of bound and continuum states, reduced transition probabilities, phase-shifts, photo-disintegration cross sections, radiative capture cross sections, and astrophysical S-factors, for a two-body nuclear system. The code is based on a potential model of a Woods-Saxon, a Gaussian, or a M3Y, type. It can be used to calculate nuclear reaction rates in numerous astrophysical scenarios.

PACS numbers: 25.40.Lw,25.20.-x, 26

Keywords: Astrophysical S-factor, photo-disintegration, potential model

---

[*]Electronic address: `bertulani@nscl.msu.edu`

PROGRAM SUMMARY

1. *Title of program:* RADCAP (RADiative CApture)

   Computers: The code has been created on an IBM-PC, but also runs on UNIX machines.

   Operating systems: WINDOWS or UNIX

   Program language used: Fortran-77

   Memory required to execute with typical data: 8 Mbytes of RAM memory and 2 MB of hard disk space

   No. of bits in a word: 32 or 64

   Memory required for test run with typical data: 2 MB

   No. of lines in distributed program, including test data, etc.: 3054

   Distribution format: ASCII

   Keywords: Potential model; Photodissociation; Radiative capture; Astrophysical S-factors

   Nature of physical problem: The program calculates bound and continuum wavefunctions, phase-shifts and resonance widths, astrophysical S-factors, and other quantities of interest for direct capture reactions.

   Method of solution: Solves the radial Schrödinger equation for bound and for continuum states. First the eigenenergy is estimated by using the WKB method. Then, a Numerov integration is used outwardly and inwardly and a matching at the nuclear surface is done to obtain the energy and the bound state wavefunction with good accuracy. The continuum states are obtained by a Runge-Kutta integration, matching the Coulomb wavefunctions at large distances outside the range of the nuclear potential.

   Typical running time: Almost all the CPU time is consumed by the solution of the radial Schrödinger equation. It is about 1 min on a 1GHz Intel P4-processor machine for a Woods-Saxon potential.

LONG WRITE-UP

I. INTRODUCTION

In astrophysically relevant nuclear reactions two opposite reaction mechanisms are of importance, compound–nucleus formation and direct reactions (for more details, see, e.g., [1]). At the low reaction energies occurring in primordial and stellar nucleosynthesis the direct mechanism cannot be neglected and can even be dominant. The reason for this behavior is that only a few levels exist for low excitations of the compound nucleus.

In order to calculate the direct capture cross sections one needs to solve the many body problem for the bound and continuum states of relevance for the capture process. There are several levels of difficulty in attacking this problem. The simplest solution is based on a potential model to obtain single-particle energies and wavefunctions. In numerous situations this solution is good enough to obtain the cross sections within the accuracy required to reproduce the experiments.

In this article a computer program is described which aims at calculating direct capture cross sections, based on a potential model. The program calculates bound and continuum wavefunctions, phase-shifts, energy location of resonances, as well as the particle-decay width, photodisintegration cross sections, radiative capture cross sections and astrophysical S-factors. The formalism for this model has been developed in Refs. [2–4].

II. BOUND STATES

The computer code RADCAP calculates various quantities of interest for two-body fusion reactions of the type

$$a + b \longrightarrow c + \gamma, \quad \text{or} \quad a\,(b,\gamma)\,c \ . \tag{1}$$

The internal structure of the nuclei a and b is not taken into account. Thus, the states of the nucleus c is obtained by the solution of the Schrödinger equation for the relative motion of a and b in a nuclear + Coulomb potential. Particles a, b, and c have intrinsic spins labelled by I_a, I_b and J, respectively. The corresponding magnetic substates are labelled by M_a, M_b and M. The orbital angular momentum for the relative motion of $a+b$ is described by l and m. In most situations of interest, the particle b is a nucleon and a is a "core" nucleus. Thus

it is convenient to couple angular momenta as $\mathbf{l} + \mathbf{I}_b = \mathbf{j}$ and $\mathbf{j} + \mathbf{I}_a = \mathbf{J}$, where $\mathbf{J}$ is called the channel spin. Below we also use the notation $\mathbf{s}$, instead of $\mathbf{I}_b$, for the intrinsic spin of particle b.

The bound state wavefunctions of c are specified by

$$\Psi_{JM}(\mathbf{r}) = \frac{u_{lj}^J(r)}{r} \mathcal{Y}_{JM}^l , \tag{2}$$

where r is the relative coordinate of a and b, $u_{lj}^J(r)$ is the radial wavefunction and $\mathcal{Y}_{JM}^l$ is the spin-angle wavefunction

$$\mathcal{Y}_{JM}^l = \sum_{m, M_a} \langle jmI_aM_a|JM\rangle |jm\rangle |I_aM_a\rangle, \quad \text{with} \quad |jm\rangle = \sum_{m_l, M_b} Y_{lm_l}(\widehat{\mathbf{r}}) \chi_{M_b} \tag{3}$$

where χ_{M_b} is the spinor wavefunction of particle b and $\langle jmI_aM_a|JM\rangle$ is a Clebsch-Gordan coefficient.

The ground-state wavefunction is normalized so that

$$\int d^3r \ |\Psi_{JM}(\mathbf{r})|^2 = \int_0^\infty dr \ |u_{lj}^J(r)|^2 = 1. \tag{4}$$

The wavefunctions are calculated using a spin-orbit potential of the form

$$V(\mathbf{r}) = V_0(r) + V_S(r) \ (\mathbf{l}.\mathbf{s}) + V_C(r) \tag{5}$$

where $V_0(r)$ and $V_S(r)$ are the central and spin-orbit interaction, respectively, and $V_C(r)$ is the Coulomb potential of a uniform distribution of charges:

$$\begin{aligned} V_C(r) &= \frac{Z_aZ_be^2}{r} \quad \text{for} \quad r > R_C \\ &= \frac{Z_aZ_be^2}{2R_C}\left(3 - \frac{r^2}{R_C^2}\right) \quad \text{for} \quad r < R_C, \end{aligned} \tag{6}$$

where Z_i is the charge number of nucleus $i = a, b$.

One can use two kinds of approach to build up the potentials $V_0(r)$ and $V_S(r)$. In a Woods-Saxon parametrization they are given by

$$V_0(r) = V_0 \ f_0(r), \quad \text{and} \quad V_S(r) = -V_{S0} \left(\frac{\hbar}{m_\pi c}\right)^2 \frac{1}{r}\frac{d}{dr}f_S(r)$$

$$\text{with} \quad f_i(r) = \left[1 + \exp\left(\frac{r - R_i}{a_i}\right)\right]^{-1}. \tag{7}$$

The spin-orbit interaction in Eq. 7 is written in terms of the pion Compton wavelength, $\hbar/m_\pi c = 1.414$ fm. The parameters V_0, V_{S0}, R_0, a_0, R_{S0}, and a_{S0} are adjusted so that the ground state energy E_B (or the energy of an excited state) is reproduced.

Alternatively, and perhaps more adequate for some situations, one can construct the potentials using a more microscopic approach. Among these models, the M3Y interaction is very popular. It has been shown to work quite reasonably for elastic and inelastic scattering of heavy ions at low and intermediate energy nuclear collisions [5, 6]. It has been applied to calculations of radiative capture cross sections with relative success (see, e.g., [7]).

In its simplest form the M3Y interaction is given by two direct terms with different ranges, and an exchange term represented by a delta interaction:

$$t(s) = A\frac{e^{-\beta_1 s}}{\beta_1 s} + B\frac{e^{-\beta_2 s}}{\beta_2 s} + C\delta(s) \, , \tag{8}$$

where one of the possible set for these parameters is given by [5, 6] $A = 7999$ MeV, $B = -2134$ MeV, $C = -276$ MeV fm^3, $\beta_1 = 4$ fm^{-1}, and $\beta_2 = 2.5$ fm^{-1}.

The central part of the potential is obtained by a folding of this interaction with the ground state densities, ρ_a and ρ_b, of the nuclei a and b:

$$V_0^{M3Y}(r) = \lambda_0 V^{M3Y}(r) = \lambda_0 \int d^3r_1 \, d^3r_2 \, \rho_a(r_1)\rho_b(r_2) \, t(s) \, , \tag{9}$$

with $s = |\mathbf{r} + \mathbf{r}_2 - \mathbf{r}_1|$. λ_0 is a normalization factor which is close to unity. We assume that the densities ρ_i are spherically symmetric. The nuclear densities can be taken from e.g. Ref. [8] for the charge matter densities. To obtain the matter density one can use the relation $\langle r_m^2 \rangle^{1/2} = \sqrt{\langle r_{ch}^2 \rangle - (0.85)^2}$, where $\langle r_{ch}^2 \rangle^{1/2}$ and $\langle r_m^2 \rangle^{1/2}$ are the charge and matter rms radii of the nucleus and the proton radius is taken as 0.85 fm.

The spin-orbit part of the optical potential is parametrized as

$$V_S^{M3Y}(r) = -\lambda_{S0} \left(\frac{\hbar}{m_\pi c}\right)^2 \frac{1}{r} \frac{d}{dr} V^{M3Y}(r). \tag{10}$$

The bound-state wavefunctions are calculated by solving the radial Schrödinger equation

$$-\frac{\hbar^2}{2m_{ab}} \left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2}\right] u_{lj}^J(r) + [V_0(r) + V_C(r) + \langle \mathbf{s}.\mathbf{l}\rangle \, V_{S0}(r)] u_{lj}^J(r) = E_i u_{lj}^J(r) \tag{11}$$

where $\langle \mathbf{s}.\mathbf{l}\rangle = [j(j+1) - l(l+1) - s(s+1)]/2$. This equation must satisfy the boundary conditions $u_{lj}^J(r=0) = u_{lj}^J(r=\infty) = 0$ which is only possible for discrete energies E corresponding to the bound states of the nuclear + Coulomb potential.

III.   CONTINUUM STATES

The continuum wavefunctions are calculated with the potential model as described above. The parameters are often not the same as the ones used for the bound states. The continuum states are now identified by the notation $u_{Elj}^J(r)$, where the (continuous) energy E is related to the relative momentum k of the system $a+b$ by $E = \hbar^2 k^2/2m_{ab}$.

The radial equation to be solved is the same as Eq. 11, but with the boundary conditions at infinity replaced by (see, e.g, Ref. [9])

$$u_{Elj}^J(r \longrightarrow \infty) = i\sqrt{\frac{m_{ab}}{2\pi k \hbar^2}} \left[H_l^{(-)}(r) - S_{lJ} H_l^{(+)}(r) \right] e^{i\sigma_l(E)} \tag{12}$$

where $S_{lJ} = \exp\left[2i\delta_{lJ}(E)\right]$, with $\delta_{lJ}(E)$ being the nuclear phase-shift and $\sigma_l(E)$ the Coulomb one, and

$$H_l^{(\pm)}(r) = G_l(r) \pm iF_l(r) \ . \tag{13}$$

F_l and G_l are the regular and irregular Coulomb wavefunctions. If the particle b is not charged (e.g., a neutron) the Coulomb functions reduce to the usual spherical Bessel functions, $j_l(r)$ and $n_l(r)$.

At a conveniently chosen large distance $r = R$, outside the range of the nuclear potential, one can define the logarithmic derivative

$$\alpha_{lJ} = \left(\frac{du_{Elj}^J/dr}{u_{Elj}^J}\right)_{r=R} . \tag{14}$$

The phaseshifts $\delta_{lJ}(E)$ are obtained by matching the logarithmic derivative with the asymptotic value obtained with the Coulomb wavefunctions. This procedure yields

$$S_{lJ} = \frac{G_l' - iF_l' - \alpha_{lJ}\ (G_l - iF_l)}{G_l' + iF_l' - \alpha_{lJ}\ (G_l + iF_l)}, \tag{15}$$

where the primes mean derivation with respect to the radial coordinate at the position R.

The continuum wavefunctions are normalized so as to satisfy the relation

$$\left\langle u_{Elj}^J | u_{E'l'j'}^{J'} \right\rangle = \delta(E - E')\, \delta_{JJ'} \delta_{jj'} \delta_{ll'}, \tag{16}$$

what means, in practice, that the continuum wavefunctions $u_{Elj}(r)$ are normalized to $-\sqrt{2m_{ab}/\pi\hbar^2 k}\ e^{i\delta_{lJ}} \sin(kr + \delta_{lJ})$ at large r.

A resonance in a particular channel lJ is characterized by

$$\left.\frac{d^2\delta_{lJ}}{dE^2}\right|_{E_{lJ}^R} = 0, \qquad \text{and} \qquad \left.\frac{d\delta_{lJ}}{dE}\right|_{E_{lJ}^R} > 0 \ . \tag{17}$$

6

The single-particle width of the resonance can be calculated from

$$\Gamma_{lJ}^R = 2 \left(\frac{d\delta_{lJ}}{dE} \bigg|_{E_{lJ}^R} \right)^{-1}. \tag{18}$$

IV. MULTIPOLE MATRIX ELEMENTS

The operators for electric transitions of multipolarity $\lambda\pi$ are given by (see, e.g. Ref. [11])

$$\mathcal{O}_{E\lambda\mu} = e_\lambda \, r^\lambda Y_{\lambda\mu}\left(\widehat{\mathbf{r}}\right), \tag{19}$$

where the effective charge, which takes into account the displacement of the center-of-mass, is

$$e_\lambda = Z_b e \left(-\frac{m_a}{m_c} \right)^\lambda + Z_a e \left(\frac{m_b}{m_c} \right)^\lambda. \tag{20}$$

For magnetic dipole transitions

$$\mathcal{O}_{M1\mu} = \sqrt{\frac{3}{4\pi}} \mu_N \left[e_M l_\mu + \sum_{i=a,b} g_i \left(s_i \right)_\mu \right], \qquad e_M = \left(\frac{m_a^2 Z_a}{m_c^2} + \frac{m_b^2 Z_b}{m_c^2} \right), \tag{21}$$

where l_μ and s_μ are the spherical components of order μ ($\mu = -1, 0, 1$) of the orbital and spin angular momentum ($\mathbf{l} = -i\mathbf{r} \times \nabla$, and $\mathbf{s} = \sigma/2$) and g_i are the gyromagnetic factors of particles a and b. The nuclear magneton is given by $\mu_N = e\hbar/2m_N c$.

The matrix element for the transition $J_0 M_0 \longrightarrow JM$, using the convention of Ref. [11], is given by

$$\langle JM \left| \mathcal{O}_{E\lambda\mu} \right| J_0 M_0 \rangle = \langle J_0 M_0 \lambda\mu | JM \rangle \frac{\langle J \| \mathcal{O}_{E\lambda} \| J_0 \rangle}{\sqrt{2J+1}}. \tag{22}$$

From the single-particle wavefunctions one can calculate the reduced matrix elements $\langle lj \| \mathcal{O}_{E\lambda} \| l_0 j_0 \rangle_J$. The subscript J is a reminder that the matrix element depends on the channel spin J, because one can use different potentials in the different channels. The reduced matrix element $\langle J \| \mathcal{O}_{E\lambda} \| J_0 \rangle$ can be obtained from a standard formula of angular momentum algebra, e.g. Eq. (7.17) of Ref. [12]. One gets

$$\langle J \| \mathcal{O}_{E\lambda} \| J_0 \rangle = (-1)^{j+I_a+J_0+\lambda} \left[(2J+1)(2J_0+1) \right]^{1/2} \begin{Bmatrix} j & J & I_a \\ J_0 & j_0 & \lambda \end{Bmatrix} \langle lj \| \mathcal{O}_{E\lambda} \| l_0 j_0 \rangle_J. \tag{23}$$

To obtain $\langle lj \| \mathcal{O}_{E\lambda} \| l_0 j_0 \rangle_J$ one needs the matrix element $\langle lj \| r^\lambda Y_\lambda \| l_0 j_0 \rangle_J$ for the spherical harmonics, e.g. Eq. (A2.23) of Ref. [13]. For $l_0 + l + \lambda = $ even, the result is

$$\langle lj \| \mathcal{O}_{E\lambda} \| l_0 j_0 \rangle_J = \frac{e_\lambda}{\sqrt{4\pi}} (-1)^{l_0+l+j_0-j} \frac{\hat{\lambda}\hat{j}_0}{\hat{j}} < j_0 \tfrac{1}{2} \lambda 0 | j \tfrac{1}{2} > \int_0^\infty dr \, r^\lambda \, u_{lj}^J(r) \, u_{l_0 j_0}^{J_0}(r), \tag{24}$$

7

where we use here the notation $\widehat{k} = \sqrt{2k+1}$, and $\widetilde{k} = \sqrt{k(k+1)}$. For $l_0 + l + \lambda = $ odd, the reduced matrix element is null.

Eqs. 22 and 23 can also be used for the magnetic dipole excitations. In comparison with the electric dipole transitions their cross sections are reduced by a factor of v^2/c^2, where v is the relative velocity of the $a+b$ system. At very low energies, $v \ll c$, and the $M1$ transitions will be much smaller than the electric transitions. Only in the case of sharp resonances, the M1 transitions play a role, e.g. for the $J = 1^+$ state in ^{8}B at $E_R = 630$ keV above the proton separation threshold [4, 14]. However, the potential model apparently is not good in reproducing the M1 transition amplitudes [15]. We only treat here the case in which the particle b is a nucleon. For that one needs the reduced matrix elements $\left\langle lj \left\| \widehat{l} \right\| l_0 j_0 \right\rangle_J$ and $\langle lj \| \widehat{\sigma} \| l_0 j_0 \rangle_J$ which are, e.g., given by Eqs. (A2.20) and (A2.19) of Ref. [13]. For $l = l_0$ one obtains

$$
\langle lj \| \mathcal{O}_{M1} \| l_0 j_0 \rangle_J = (-1)^{j+I_a+J_0+1} \sqrt{\frac{3}{4\pi}} \, \widehat{J}\widehat{J}_0 \left\{ \begin{array}{ccc} j & J & I_a \\ J_0 & j_0 & 1 \end{array} \right\} \mu_N
$$

$$
\times \left\{ \frac{1}{\widetilde{l}_0} e_M \left[\frac{2\widetilde{j}_0}{\widehat{l}_0} \left(l_0 \delta_{j_0, \, l_0+1/2} + (l_0+1)\delta_{j_0, \, l_0-1/2} \right) + (-1)^{l_0+1/2-j} \frac{\widehat{j}_0}{\sqrt{2}} \delta_{j_0, \, l_0 \pm 1/2} \delta_{j, \, l_0 \mp 1/2} \right] \right.
$$

$$
+ g_N \frac{1}{\widehat{l}_0^2} \left[(-1)^{l_0+1/2-j_0} \widetilde{j}_0 \delta_{j, \, j_0} - (-1)^{l_0+1/2-j} \frac{\widehat{j}_0}{\sqrt{2}} \delta_{j_0, \, l_0 \pm 1/2} \delta_{j, \, l_0 \mp 1/2} \right]
$$

$$
+ g_a (-1)^{I_a+j_0+J+1} \widehat{J}_0 \widetilde{J} \widehat{I}_a \widetilde{I}_a \left\{ \begin{array}{ccc} I_a & J & j_0 \\ J_0 & I_a & 1 \end{array} \right\} \right\} \int_0^\infty dr \, u_{lj}^J(r) \, u_{l_0 j_0}^{J_0}(r), \tag{25}
$$

The spin g-factor is $g_N = 5.586$ for the proton and $g_N = -3.826$ for the neutron. The magnetic moment of the core nucleus is given by $\mu_a = g_a \mu_N$. If $l \neq l_0$ the magnetic dipole matrix element is zero.

V. THE ASTROPHYSICAL S-FACTOR

The multipole strength, or response functions, for a particular partial wave, summed over final channel spins, is defined by

$$\frac{dB\left(\pi\lambda;\ l_0 j_0 \longrightarrow klj\right)}{dk} = \sum_J \frac{\left|\langle kJ \left\|\mathcal{O}_{\pi\lambda}\right\| J_0\rangle\right|^2}{2J_0 + 1}$$

$$= \sum_J (2J+1) \left\{ \begin{matrix} j & J & I_a \\ J_0 & j_0 & \lambda \end{matrix} \right\}^2 \left|\langle klj \left\|\mathcal{O}_{\pi\lambda}\right\| l_0 j_0\rangle_J\right|^2, \qquad (26)$$

where $\pi = E$, or M.

If the matrix elements are independent of the channel spin, this sum reduces to the usual single-particle strength $\left|\langle klj \left\|\mathcal{O}_{\pi\lambda}\right\| l_0 j_0\rangle\right|^2 / (2j_0 + 1)$. For transitions between the bound states the same formula as above can be used to obtain the reduced transition probability by replacing the continuum wavefunctions $u_{klj}^J(r)$ by the bound state wavefunction $u_{lj}^J(r)$. That is,

$$B\left(\pi\lambda;\ l_0 j_0 J_0 \longrightarrow lj J\right) = (2J+1) \left\{ \begin{matrix} j & J & I_a \\ J_0 & j_0 & \lambda \end{matrix} \right\}^2 \left|\langle lj \left\|\mathcal{O}_{\pi\lambda}\right\| l_0 j_0\rangle\right|^2. \qquad (27)$$

For bound state to continuum transitions the total multipole strength is obtained by summing over all partial waves,

$$\frac{dB\left(\pi\lambda\right)}{dE} = \sum_{lj} \frac{dB\left(\pi\lambda;\ l_0 j_0 \longrightarrow klj\right)}{dE}. \qquad (28)$$

The differential form of the response function in terms of the momentum E is a result of the normalization of the continuum waves according to Eq. 12.

The photo-absorption cross section for the reaction $\gamma + c \longrightarrow a + c$ is given in terms of the response function by [10]

$$\sigma_\gamma^{(\lambda)}\left(E_\gamma\right) = \frac{(2\pi)^3 (\lambda+1)}{\lambda\left[(2\lambda+1)!!\right]^2} \left(\frac{m_{ab}}{\hbar^2 k}\right) \left(\frac{E_\gamma}{\hbar c}\right)^{2\lambda-1} \frac{dB\left(\pi\lambda\right)}{dE}, \qquad (29)$$

where $E_\gamma = E + |E_B|$, with $|E_B|$ being the binding energy of the $a+b$ system. For transitions between bound states, one has

$$\sigma_\gamma^{(\pi\lambda)}\left(E_\gamma\right) = \frac{(2\pi)^3 (\lambda+1)}{\lambda\left[(2\lambda+1)!!\right]^2} \left(\frac{E_\gamma}{\hbar c}\right)^{2\lambda-1} B\left(\pi\lambda;\ l_0 j_0 J_0 \longrightarrow lj J\right) \delta\left(E_f - E_i - E_\gamma\right), \qquad (30)$$

where E_i (E_f) is the energy of the initial (final) state.

The cross section for the radiative capture process $a + b \longrightarrow c + \gamma$ can be obtained by detailed balance [10], and one gets

$$\sigma_{(\pi\lambda)}^{(\text{rc})}(E) = \left(\frac{E_\gamma}{\hbar c}\right)^{2\lambda-1} \frac{2(2I_c+1)}{(2I_a+1)(2I_b+1)} \sigma_\gamma^{(\lambda)}(E_\gamma). \tag{31}$$

The total capture cross section σ_{nr} is determined by the capture to all bound states with the single particle spectroscopic factors $C^2 S_i$ in the final nucleus

$$\sigma_{\text{nr}}(E) = \sum_{i,\pi,\lambda} (C^2 S)_i \; \sigma_{(\pi\lambda),i}^{(\text{rc})}(E). \tag{32}$$

Experimental information or detailed shell model calculations have to be performed to obtain the spectroscopic factors $(C^2 S)_i$. For example, the code OXBASH [16] can used for this purpose.

For charged particles the astrophysical S-factor for the direct capture from a continuum state to the bound state is defined as

$$S^{(c)}(E) = E \; \sigma_{\text{nr}}(E) \; \exp\left[2\pi\eta(E)\right], \qquad \text{with} \qquad \eta(E) = Z_a Z_b e^2/\hbar v, \tag{33}$$

where v is the relative velocity between a and b.

VI. NUCLEAR REACTION RATES IN STELLAR ENVIRONMENTS

The nuclear reaction rate, measuring the number of reactions per particle pair, $a + b$, per second in the stellar environment can be calculated from the nuclear cross section σ for a given reaction by folding it with the velocity distribution of the particles involved. In most astrophysical applications the nuclei are in a thermalized plasma, yielding a Maxwell-Boltzmann velocity distribution. The astrophysical reaction rate R at a temperature T can then be written as [17]

$$R(T) = \frac{n_a n_b}{1 + \delta_{ab}} \langle \sigma v \rangle, \tag{34}$$

where n_i is the number density of the nuclear species i. The denominator takes care of the special case of two identical nuclei in the entrance channel. The quantity $\langle \sigma v \rangle$ is given by

$$\langle \sigma v \rangle = \left(\frac{8}{\pi m_{ab}}\right)^{1/2} \frac{1}{(k_{\text{B}}T)^{3/2}} \int_0^\infty \sigma(E) \; E \; \exp\left(-\frac{E}{k_{\text{B}}T}\right) dE, \tag{35}$$

with k_B the Boltzmann constant.

The threshold behavior of radiative capture cross sections is fundamental in nuclear astrophysics because of the small projectile energies in the thermonuclear region. For example, for neutron capture near the threshold the cross section can be written [10] as

$$\sigma_{if} = \frac{\pi}{k^2} \frac{-4kR \operatorname{Im}\alpha_0}{|\alpha_0|^2} \; , \tag{36}$$

where α_0 is the logarithmic derivative for the s wave, given by Eq. 14. Since α_0 is only weakly dependent on the projectile energy, one obtains for low energies the well–known $1/v$–behavior.

With increasing neutron energy higher partial waves with $l > 0$ contribute more significantly to the radiative capture cross section. Thus the product σv becomes a slowly varying function of the neutron velocity and one can expand this quantity in terms of v or $\sqrt{E}$ around zero energy:

$$\sigma v = S^{(n)}(0) + \dot{S}^{(n)}(0)\sqrt{E} + \frac{1}{2}\ddot{S}^{(n)}(0)E + \dots \; . \tag{37}$$

The quantity $S^{(n)}(E) = \sigma v$ is the astrophysical S–factor for neutron–induced reactions and the dotted quantities represent derivatives with respect to $E^{1/2}$, i.e., $\dot{S}^{(n)} = 2\sqrt{E}\frac{dS^{(n)}}{dE}$ and $\ddot{S}^{(n)} = 4E \frac{d^2 S^{(n)}}{dE^2} + 2 \frac{dS^{(n)}}{dE}$. Notice that the above astrophysical S–factor for neutron–induced reactions is different from that for charged–particle induced reactions. In the astrophysical S–factor for charged–particle induced reactions also the penetration factor through the Coulomb barrier has to be considered (Eq. 33).

Inserting this into Eq. 35 we obtain for the reaction rate for neutron–induced reactions

$$\langle \sigma v \rangle = S(0) + \left(\frac{4}{\pi}\right)^{\frac{1}{2}} \dot{S}(0)(k_B T)^{\frac{1}{2}} + \frac{3}{4}\ddot{S}(0)k_B T + \dots \; . \tag{38}$$

In most astrophysical neutron–induced reactions, neutron s–waves will dominate, resulting in a cross section showing a $1/v$–behavior (i.e., $\sigma(E) \propto 1/\sqrt{E}$). In this case, the reaction rate will become independent of temperature, $R = \text{const}$. Therefore it will suffice to measure the cross section at one temperature in order to calculate the rates for a wider range of temperatures. The rate can then be computed very easily by using

$$R = \langle \sigma v \rangle = \langle \sigma \rangle_T \, v_T = \text{const} \; , \tag{39}$$

with

$$v_T = \left(\frac{2kT}{m}\right)^{1/2} \; . \tag{40}$$

The mean lifetime τ_n of a nucleus against neutron capture, i.e., the mean time between subsequent neutron captures is inversely proportional to the available number of neutrons n_n and the reaction rate $R_{n\gamma}$:

$$\tau_n = \frac{1}{n_n R_{n\gamma}} \ .$$ (41)

If this time is shorter than the beta–decay half–life of the nucleus, it will be likely to capture a neutron before decaying (r-process). In this manner, more and more neutrons can be captured to build up nuclei along an isotopic chain until the beta–decay half–life of an isotope finally becomes shorter than τ_n. With the very high neutron densities encountered in several astrophysical scenarios, isotopes very far–off stability can be synthesized.

For low $|E_B|$-values, e.g. for halo-nuclei, the simple $1/v$-law does not apply anymore. A significant deviation can be observed if the neutron energy is of the order of the $|E_B|$-value. In this case the response function in Eq. 28 can be calculated analytically under simplifying assumptions (see Ref.[18]). For direct capture to weakly bound final states, the bound–state wave function $u_{lj}(r)$ decreases very slowly in the nuclear exterior, so that the contributions come predominantly from far outside the nuclear region, i.e., from the *nuclear halo*. For this asymptotic region the scattering and bound wave functions in Eq. 2 can be approximated by their asymptotic expressions neglecting the nuclear potential [19]

$$u_l(kr) \propto j_l(kr), \qquad u_{l_0}(r) \propto h_{l_0}^{(+)}(i\eta r) \ ,$$

where j_l and $h_{l_0}^{(+)}$ are the spherical Bessel, and the Hankel function of the first kind, respectively. The separation energy $|E_B|$ in the exit channel is related to the parameter η by $|E_B| = \hbar^2 \eta^2 / (2m_{ab})$.

Performing the calculations of the radial integrals in Eq. 24, one readily obtains the energy dependence of the radiative capture cross section for halo nuclei [18, 19]. For example, for a transition s$\longrightarrow$p it becomes

$$\sigma_{(E1)}^{(rc)}(\mathrm{s} \to \mathrm{p}) \propto \frac{1}{\sqrt{E}} \frac{(E + 3|E_B|)^2}{E + |E_B|} \ ,$$ (42)

while a transition p$\to$s has the energy dependence

$$\sigma_{(E1)}^{(rc)}(\mathrm{p} \to \mathrm{s}) \propto \frac{\sqrt{E}}{E + |E_B|} \ .$$ (43)

If $E \ll |E_B|$ the conventional energy dependence is recovered. From the above equations one obtains that the reaction rate is not constant (for s-wave capture) or proportional to T

12

(for p-wave capture) in the case of small $|E_B|$-values. These general analytical results can be used as a guide for interpreting the numerical calculations involving neutron halo nuclei.

In the case of charged particles $S(E)$ is expected to be a slowly varying function in energy for non-resonant nuclear reactions. In this case, $S(E)$ can be expanded in a McLaurin series,

$$S(E) = S(0) + \dot{S}(0)E + \frac{1}{2}\ddot{S}(0)E^2 + \cdots \tag{44}$$

Using this expansion in Eq. 35 and approximating the product of the exponentials $\exp(-E/k_\mathrm{B}T)$ and $\exp[2\pi\eta(E)]$ by a Gaussian centered at the energy E_0, Eq. 35 can be evaluated as [1]

$$\langle\sigma v\rangle = \left(\frac{2}{m_{ab}}\right)^{1/2}\frac{\Delta}{(kT)^{3/2}}\,S_{\mathrm{eff}}(E_0)\exp\left(-\frac{3E_0}{kT}\right) \tag{45}$$

with

$$S_{\mathrm{eff}}(E_0) = S(0)\left[1 + \frac{5}{12\tau} + \frac{\dot{S}(0)}{S(0)}\left(E_0 + \frac{35E_0}{12\tau}\right) + \frac{\ddot{S}(0)}{2S(0)}\left(E_0^2 + \frac{89E_0^2}{12\tau}\right)\right] . \tag{46}$$

The quantity E_0 defines the effective mean energy for thermonuclear fusion reactions at a given temperature T,

$$E_0 = 1.22\left(Z_a^2 Z_b^2 m_{ab}T_6^2\right)^{1/2}\quad\mathrm{keV}\ , \tag{47}$$

where T_6 measures the temperature in 10^6 K. The quantities τ and Δ are given by

$$\tau = \frac{3E_0}{kT},\qquad \Delta = \frac{4}{\sqrt{3}}\left(E_0 kT\right)^{1/2}\ . \tag{48}$$

An analytical insight of the cross sections and astrophysical S-factors for proton-halo nuclei can also be developed (see, e.g., Ref. [20]). However, due to the Coulomb field the expressions become more complicated. The analytical formulas for direct capture cross sections involving neutron and proton halo nuclei are very useful to interpret the results obtained in a numerical calculation.

For the case of resonances, where E_r is the resonance energy, we can approximate $\sigma(E)$ by a Breit-Wigner resonance formula [10, 21]:

$$\sigma_{\mathrm{r}}(E) = \frac{\pi\hbar^2}{2\mu E}\frac{(2J_R+1)}{(2J_a+1)(2J_b+1)}\frac{\Gamma_{\mathrm{p}}\Gamma_\gamma}{(E_{\mathrm{r}}-E)^2 + (\Gamma_{\mathrm{tot}}/2)^2}\ , \tag{49}$$

where J_R, J_a, and J_b are the spins of the resonance and the nuclei a and b, respectively, and the total width Γ_{tot} is the sum of the particle decay partial width Γ_{p} and the γ-ray partial

width Γ_γ. The particle partial width, or entrance channel width, Γ_p can be expressed in terms of the single-particle spectroscopic factor S and the single-particle width $\Gamma_{s.p.}$ of the resonance state [22]

$$\Gamma_p = C^2 S \times \Gamma_{s.p.} \, , \tag{50}$$

where C is the isospin Clebsch-Gordan coefficient. The single-particle width $\Gamma_{s.p.}$ can be calculated from the scattering phase shifts of a scattering potential with the potential parameters being determined by matching the resonance energy (see Eq. 18).

The gamma partial widths Γ_γ are calculated from the electromagnetic reduced transition probabilities $B(J_i \rightarrow J_f;L)$ which carry the nuclear structure information of the resonance states and the final bound states [23]. The reduced transition rates can be computed within the framework of the shell model.

Most of the typical transitions are M1 or E2 transitions. For these the relations are

$$\Gamma_{E2}[\text{eV}] = 8.13 \times 10^{-7} \; E_\gamma^5 \; [\text{MeV}] \;\; B(E2) \; [\text{e}^2\text{fm}^4] \tag{51}$$

and

$$\Gamma_{M1}[\text{eV}] = 1.16 \times 10^{-2} \; E_\gamma^3 \; [\text{MeV}] \; B(M1) \; [\mu_N^2] \, . \tag{52}$$

For the case of narrow resonances, with width $\Gamma \ll E_r$, the Maxwellian exponent $\exp\left(-E/k_B T\right)$ can be taken out of the integral, and one finds

$$\langle \sigma v \rangle = \left(\frac{2\pi}{m_{ab}kT}\right)^{3/2} \hbar^2 \, (\omega\gamma)_R \exp\left(-\frac{E_r}{kT}\right) \, , \tag{53}$$

where the resonance strength is defined by

$$(\omega\gamma)_R = \frac{2J_R + 1}{(2J_a + 1)(2J_b + 1)} \; (1 + \delta_{ab}) \; \frac{\Gamma_p \, \Gamma_\gamma}{\Gamma_{tot}}. \tag{54}$$

For broad resonances Eq. 35 is usually calculated numerically. An interference term has to be added. The total capture cross section is then given by [24]

$$\sigma(E) = \sigma_{nr}(E) + \sigma_r(E) + 2\left[\sigma_{nr}(E)\sigma_r(E)\right]^{1/2} \cos[\delta_R(E)] \, . \tag{55}$$

In this equation $\delta_R(E)$ is the resonance phase shift. Close to a resonance, the phase shift approaches the value $\pi/2$. Thus, close to a resonance one can use the expansion

$$\delta_R(E) \simeq \frac{\pi}{2} - (E_r - E) \left.\frac{d\delta}{dE}\right|_R \, .$$

Thus, using the definition given by Eq. 18, one has

$$\delta_{\mathrm{R}}(E) = \arctan \frac{\Gamma}{2(E - E_{\mathrm{R}})} \ . \tag{56}$$

Only the contributions with the same angular momentum of the incoming wave interfere in Eq. 55.

VII.   COMPUTER PROGRAM AND USER'S MANUAL

All nuclear quantities, either known from experiments or calculated from a model, as well as the conditions realized in the experiment, are explicitly specified as input parameters. The program RADCAP then computes the potentials, bound state energies, phase-shifts, transition probabilities, photo-dissociation cross sections and astrophysical S-factors. Besides the main program (RADCAP.FOR), it contains 5 modules (OMP_M3Y.FOR, BVALUE.FOR, EIGEN.FOR, CONT.FOR and DICAP.FOR) to compute each of the these quantities.

The units used in the program are fm (femtometer) for distances and MeV for energies. The output cross sections are given in millibarns and the S-factors in eV.b.

The program is very fast and does not require a complicated input. It asks the user the calculation one wants to perform. It is divided in 5 modules and one enters the following options when prompted on the screen:

1 - for the calculation of M3Y potential,

2 - for the calculation of energy and wavefunction of bound states,

3 - for the calculation of reduced transition probabilities between bound states,

4 - for the calculation of phase shifts and wavefunctions of continuum states,

5 - for the calculation of astrophysical S-factors, response functions, photo-dissociation, and direct capture cross sections.

For each option, a different subroutine is used: 1=OMP_M3Y, 2=EIGEN, 3=BVALUE, 4=CONT and 5=DICAP.

The inputs can be commented by using the symbol "*" at the first position of an input line.

Note that the angular momenta described in the text have the following correspondence in the program: l, l_0 (L, L0); j, j_0 (J, J0), I_a, I_b (s) (AIA, AIB), J, J_0 (AICF, AIC). The program notation for the other variables are easy to recognize.

We now make a description of test cases. The outputs of these test cases are put together in a separate files *.TXT which accompanies the code packages, together with the test input files.

A. The M3Y potential

To obtain the M3Y potential one selects the option 1. This calls the subroutine OMP_M3Y, which is in a separate file called OMP_M3Y.FOR. The input file is named M3Y.INP. If the densities are not parametrized either by a Gaussian or by a Woods-Saxon function, one can enter them in the input file DENS.INP in rows of $r \times \rho_a(r) \times \rho_b(r)$. The first line of this input file should contain only the number of points in r. The function DENS_READ will read those densities and interpolate them for use in the other routines. An example is calculation of the M3Y potential for the system p $+^7$ Be as follows. For the proton one can use a Gaussian density with radius parameter $R = 0.7$ fm. For ^{7}Be a Gaussian density parametrization can be used [8] with radius parameter $R = 1.96$. An appropriate input file is listed below.

```
***********************************************
* ******** Input of subroutine OMP_M3Y *******
* IOPT = Option for densities: = 0 Gaussian or Woods-Saxon,
*            = 1 densities entered in DENS.INP
* NPNTS = number of points in the radial mesh (< 10000)
* RMAX = maximum radius size (fm) ( < 250 fm)
* IOPT   NPTS   RMAX
   0    100    10.
* If IOPT = 0, enter density parameters (if not, comment this line with a "*")
* R1, D1 = Woods-Saxon form (radius and diffuseness)
* R2, D2 = Same but for density of nucleus 2
* For Gaussian densities, enter D1=0, or D2=0
* R1    D1    R2    D2
   0.7   0.    1.96   0.
* Mass numbers
* A1    A2
```
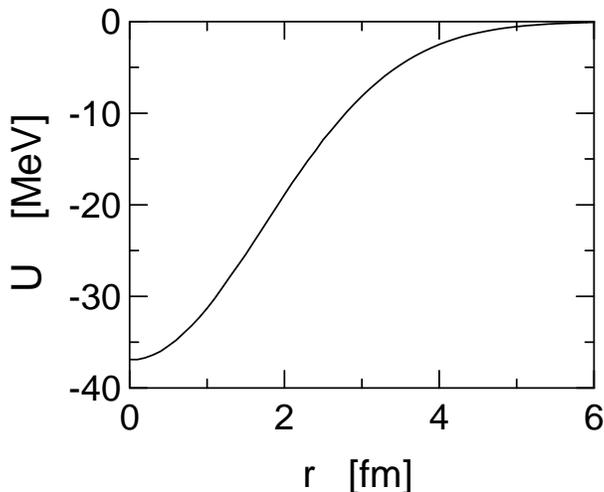
16

FIG. 1: M3Y potential for the system $p +^7$ Be.

1.   7.

****

The subroutine OMP_M3Y builds up the nuclear potential and calls the subroutine TWOFOLD which does all the work. It does the integration appearing in Eq. 9. The outputs will appear in files OMP.TXT and OMP.INP. The later one is for use as input of the M3Y potential by the other subroutines (if required). Figure 1 shows a plot of the potential obtained with this input.

The output file OMP.TXT with the input described above is provided with the package

B.   Eigenfunctions and energies

The option 2 calls the subroutine EIGEN, which is in a separate file called EIGEN.FOR. If the real part of the potential is given as an input file OMP.INP (e.g. the one generated by the subroutine OMP_M3Y) it should be written in rows of $r \times V(r)$. The first line of this input file should contain only the number of points in r. The function OMP_READ will read and interpolate the potential for use in the other routines. The subroutine DERIVATIVE calculates its derivative to be used in the calculation of Eq. 10. Let us assume we want to find the ground state of ^{8}B. The 2^+ ground state of ^{8}B can be described as a p3/2 proton coupled to the $3/2^-$ ground state ^{7}Be. The subroutine POTENT builds up the potential.

17

An example of the input file, named EIGEN.INP, which uses a Woods-Saxon potential, is shown as follows.

```
*********************************************

* ******** Input of subroutine EIGEN *******

* IOPT = option for potentials: 1 (2) for Woods-Saxon (M3Y)

* NPNTS = no. of integration points in radial coordinate ( < 10000)

* RMAX = maximum radius size ( < 250 fm)

* IOPT    NPTS    RMAX

   1    9999    250.

* N_0 = nodes of the wave function (exclude origin)

* J0 = single-particle angular momentum

* L0 = orbital angular momentum

* N_0    J0    L0

   0    1.5    1

* If IOPT = 1, enter: (if not, comment this line with a "*")

* V0 = depth of central potential

* VS0 = depth of spin-orbit potential

* R0 = radius of the potential

* AA = diffuseness of the potential

* RS0 = radius of the spin-orbit potential

* AAS = diffuseness of the spin-orbit potential

* RC = Coulomb radius (usually, RC = R0)

*_____

* WS = V_0 f(r,R0,AA) - V_S0 (l.s) (r_0^2/r) d/dr f(r,RS0,AAS)

* f(r,R0,a) = [ 1 + exp((r-R_0)/a) ]^(-1)

* r_0 = 1.4138 fm is the Compton wavelength of the pion.

*_____

* V0    R0    AA    VS0    RS0    AAS    RC

   -44.658    2.391    0.52    -9.8    2.391    0.52    2.391

* If IOPT = 2, or else (but not 1), enter FC, FSO and RC

* (in this case, insert a "*" in the above row, or delete it)

* FC = multiplicative factor of central part of M3Y potential
```

* FSO = multiplicative factor of spin-orbit part of M3Y potential

* RC = Coulomb radius

* FC   FSO   RC

* 1.5   0.2   2.391

* Z1, Z2 = charges of the nuclei

* A1, A2 = masses of the nuclei (in nucleon mass units)

* Z1   A1   Z2   A2

  1.   1.   4.   7.

****

In the example input shown above the potential parameters were chosen so as to reproduce the proton separation energy in ^{8}B which is equal to 0.136 MeV. If the M3Y potential was used, an input of the parameters λ_0 (FC), λ_{SO} (FSO), and R_C in Eqs. 6, 9 and 10 is needed. Note that this input line was commented, as we did not use it.

The calculations are mainly done in the subroutine BOUNDWAVE which solves the Schrödinger equation for the bound-state problem. When Woods-Saxon potentials are used they are constructed in the routine POTENTIAL.

The output of the wavefunction will be printed in EIGEN.TXT and GSWF.INP. The later is prepared for use as input wavefunction for the subroutine BVALUE (reduced transition probabilities), or the subroutine DICAP (direct capture subroutine). The solid line in Figure 2 shows the ground state wavefunction of ^{8}B obtained with this input.

The solid curve in figure 2 corresponds to the output file EIGEN.TXT included in the package.

C.   Reduced transition probabilities

The option 3 calls the subroutine BVALUE which calculates reduced transition probabilities. This is in a separate file called BVALUE.FOR. To make and example with ^{8}B we artificially generate a p3/2, 1^+ state, with excitation energy of 90 keV. This can be obtained by changing the WS potential input of EIGEN.INP to the values shown below

* V0   R0   AA   VS0   RS0   AAS   RC

  -30.55   2.95   0.52   -8.53   2.95   0.52   2.95
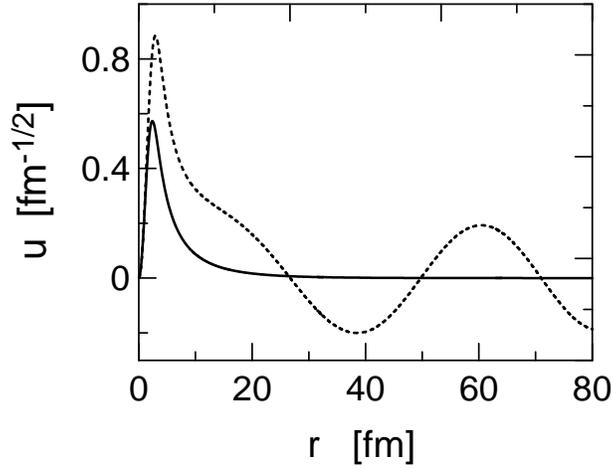
The output yields a state with energy of -0.05 MeV.

FIG. 2: The solid line shows the ground state wavefunction of ^{8}B in the potential model and the dotted line shows the real part of the wavefunction for the 1^+ resonance in ^{8}B at 630 keV (see text for details).

The input file with the option 3 is to be given in BVALUE.INP. To calculate the reduced transition probability the input file should look like the example below.

```
************************************************
* ******** Input of subroutine BVALUE *******
* AIA = spin of the particle A (core)
* AIB = intrinsic spin of the particle B
* AIC = total angular momentum of the ground state of C = A + B
* (channel spin)
* J0 = single particle angular momentum of B respective to A
* L0 = relative orbital angular momentum of the ground state
* AIA    AIB    AIC    J0    L0
   1.5    0.5    2    1..5    1
* N_1 = nodes of the excited state wave function (exclude origin)
* J = single-particle angular momentum
* L = orbital angular momentum
* AICF = spin of the excited state after all angular momentum coupling
* (channel spin)
```

* N_1   J   L   AICF

   0   1.5   1   1

* JOPT = 1 (0) if final state angular momentum, AICF, is (is not) to be

* summed over all possible values. If JOPT=1, AICF in the

* previous line can be entered as any value.

* JOPT

  0

* Z1, Z2 = charges of the nuclei

* A1, A2 = masses of the nuclei (in nucleon mass units)

* Z1   A1   Z2   A2

   1.   1.   4.   7.

* IOPT = option for potentials: 1 (2) for Woods-Saxon (M3Y)

* Integration parameters for radial wavefunctions:

* NPNTS = no. of integration points in radial coordinate (< 10000)

* RMAX = maximum radius size (250 fm)

* IOPT NPTS RMAX

   1   9999   250.

* V0 = depth of central potential

* R0 = radius of the central potential

* AA = diffuseness of the central potential

* VS0 = depth of spin-orbit potential

* RS0 = radius of the spin-orbit potential

* AAS = diffuseness of the spin-orbit potential

* RC = Coulomb radius (usually, RC = R0)

*_____

* WS = V_0 f(r,R0,AA) - V_S0 (l.s) (r_0^2/r) d/dr f(r,RS0,AAS)

* f(r,R0,a) = [1 + exp((r-R_0)/a)]^(-1)

* r_0 = 1.4138 fm is the Compton wavelength of the pion.

* (if IOPT=2, comment the input line with a "*")

*_____

* V0   R0   AA   VS0   RS0   AAS   RC

   -30.55   2.95   0.52   -8.53   2.95   0.52   2.95

* If IOPT = 2, or else (but not 1), enter FC, FSO and RC:

* (in this case, insert a '*' sign in above row, or delete it)

* FC = multiplicative factor of central part of M3Y potential

* FSO = multiplicative factor of spin-orbit part of M3Y potential

* RC = Coulomb radius

* (if IOPT=1, comment the input line with a "*")

* FC   FSO   RC

* 1.5   0.2   2.391

* MP = multipolarity: 0 (M1), 1 (E1), 2 (E2)

* MP

  2

* GA = magnetic moment (in units of the nuclear magneton) of

* particle A (core)

* GB = magnetic moment of particle B

* GA   GB

  2.79   -1.7

****

The output of this run yields $B(E2; \ i \longrightarrow f) = 3.76$ e^2 fm^4. The spectroscopic factors for the initial and final states are taken as the unity. If they are known one just multiply this result by their corresponding values.

The output file BVALUE.TXT with the input described above is provided with the package.

The bound state is calculated by the routine BOUNDWAVE and the 3-j and 6-j coefficients are calculated in the routines THREEJ and SIXJ, respectively.

D.   Phase-shifts and resonances

If one uses the option 4 the program will calculate the scattering phase-shifts for a given set of potential parameters and angular momentum quantum numbers for the continuum waves. This is in a separate file called CONT.FOR. For example, one might want to calculate the phase-shifts for the p+^{8}Be system in the energy interval $E = 0 - 3$ MeV. The input file CONT.INP could be written as follows.

```
*********************************************

* ********    Input of subroutine CONT     *******

* IOPT = option for potentials: 1 (2) for Woods-Saxon (M3Y)

* NPNTS = no. of integration points in radial coordinate ( < 10000)

* RMAX = maximum radius size (< 250 fm)

* NEPTS = number of points in energy ( < 1000)

* IOPT    NPNTS    RMAX    NEPTS

    1    9999    250.    200

* V0 = depth of central potential

* VS0 = depth of spin-orbit potential

* R0 = radius of the potential

* AA = diffuseness of the potential

* RS0 = radius of the spin-orbit potential

* AAS = diffuseness of the spin-orbit potential

* RC = Coulomb radius (usually RC = R0)

*_____-

* WS = V_0 f(r,R0,AA) - V_S0 (l.s) (r_0^2/r) d/dr f(r,RS0,AAS)

* f(r,R0,A) = [ 1 + exp((r-R0)/a) ]^(-1)

* r_0 = 1.4138 fm is the Compton wavelength of the pion.

* (if IOPT=2, comment the input line with a "*")

*_____-

* V0    R0    AA    VS0    RS0    AAS    RC

   -42.3    2.391    0.52    -9.8    2.391    0.52    2.391

* If IOPT = 2, or else (but not 1), enter FC, FSO and RC:

* (in this case, insert a '*' sign in above row, or delete it)

* FC = multiplicative factor of central part of M3Y potential

* FSO = multiplicative factor of spin-orbit part of M3Y potential

* RC = Coulomb radius

* (if IOPT=1, comment the input line with a "*")

* FC    FSO    RC

* 1.5    0.2    2.391
```

* Z1, Z2 = charges of the nuclei

* A1, A2 = masses of the nuclei (in nucleon mass units)

* Z1   A1   Z2   A2

   1.   1.   4.   7.

* EI, EF = initial energy, final energy

* L, J = orbital angular momentum, angular momentum j (l+s)

* EI   EF   L   J

   0.   3.   1   1.5

****

A run with this input file will show the presence of a sharp resonance at 631 keV with a width of approximately 50 keV. As for the case of bound states, the same resonance can be obtained with a different set of WS potential parameters, e.g. with the parameters shown below.

* V0   R0   AA   VS0   RS0   AAS   RC

   -28.65   2.95   0.52   -8.5   2.95   0.52   2.95

The continuum states are calculated by the subroutine CONTWAVE and the Coulomb wavefunctions are calculated by the subroutine COULOMB.

The dashed curve in Figure 2 corresponds to the output file CWAVE.TXT with the input described above and provided with the package.

The phase-shifts and their derivatives with respect to energy are printed in the output file CONT.TXT, listed in M3Y.TXT. The Figure 3 shows these quantities for the test case above.

The program also allows for the output of the continuum wavefunction for a given energy. The output of the wavefunction is printed in CWAVE.TXT. The real part of the continuum wave function of the 1^+ resonance state at 630 keV is shown in Figure 2 (dotted line).

E.   Direct capture cross sections

By choosing the option 5 the program calculates the direct capture cross sections and related quantities. This is in a separate file called DICAP.FOR. The input file is DICAP.INP. The calculations are done in the subroutine DICAP. The output files are DICAP.TXT where the strength functions (in units of e^2 $fm^{2\lambda}$), photodissociation cross sections (in mb), direct capture cross sections (in mb), and the astrophysical S-factors (in eV.b) are printed; DICAPL.TXT where the
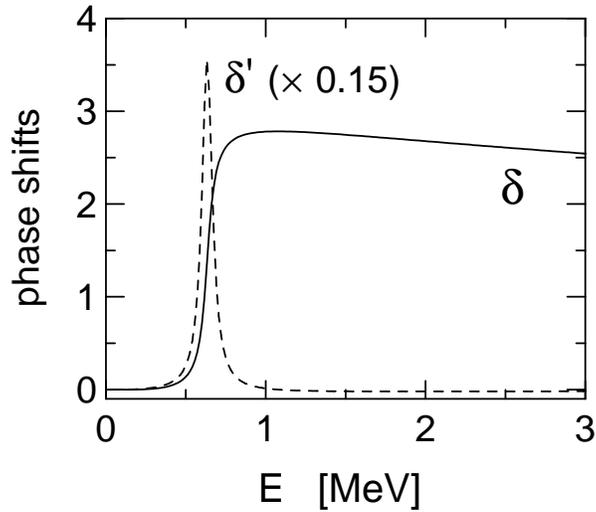
24

FIG. 3: Phase-shift (solid line) and its derivative (dashed line) for the p+^{7}Be system with the potential parameters described in the text. The 1$^+$ resonance at 630 keV is observed.

same output is printed, prepared for using in a plot program; and SFAC.TXT where the S-factor and its first and second derivatives with respect to the energy are printed. These can be used in the calculation of the reaction rates by using Eqs. 44, 45 and 46.

An input example is presented below.

```
**********************************************
* ******** Input of program DICAP *******
* IOPT = option for potentials: 1 (2) for Woods-Saxon (M3Y)
* NPNTS = no. of integration points in radial coordinate ( < 10000)
* RMAX = maximum radius size (< 250 fm).
* NEPTS = number of points in energy ( < 1000)
* IOPT    NPNTS    RMAX    NEPTS
   1    9999    250.    200
* N_0 = nodes of the ground state wave function
* AIA = spin of the particle A (core)
* AIB = intrinsic spin of the particle B
* AIC = total angular momentum of the ground state of C = A + B
* (channel spin)
```

* J0 = single-particle angular momentum

* L0 = orbital angular momentum

* EBOUND = binding energy of the ground state (absolute value)

* N_0   AIA   AIB   AIC   AJ0   L0   EBOUND

   0   1.5   0.5   2   1.5   1   0.14

* JOPT = 1 (0) if final state angular momentum, AICF, is (is not) to be

* summed over all possible values. If JOPT=1, AICF can be

* entered as any value.

* AICF = spin of the excited state after all angular momentum coupling

* (channel spin)

* JOPT   AICF

   1   1.

* Z1, Z2 = charges of the nuclei

* A1, A2 = masses of the nuclei (in nucleon mass units)

* Z1   A1   Z2   A2

   1.   1.   4.   7.

* V0 = depth of central potential

* R0 = radius of the central potential

* AA = diffuseness of the central potential

* VS0 = depth of spin-orbit potential

* RS0 = radius of the spin-orbit potential

* AAS = diffuseness of the spin-orbit potential

* RC = Coulomb radius (usually, RC = R0)

*_____

* WS = V_0 f(r,R0,AA) - V_S0 (l.s) (r_0^2/r) d/dr f(r,RS0,AAS)

* f(r,R0,a) = [1 + exp((r-R_0)/a)]^(-1)

* r_0 = 1.4138 fm is the Compton wavelength of the pion.

* (if IOPT=2, comment the input line with a "*")

*_____

* V0   R0   AA   VS0   RS0   AAS   RC

   -44.658   2.391   0.52   -9.8   2.391   0.52   2.391

* If IOPT = 2, or else (but not 1), enter FC, FSO and RC:

* (in this case, insert a '*' sign in above row, or delete it)

* FC = multiplicative factor of central part of M3Y potential

* FSO = multiplicative factor of spin-orbit part of M3Y potential

* RC = Coulomb radius

* (if IOPT=1, comment the input line with a "*")

* FC   FSO   RC

*   1.5   0.2   2.391

* EI,EF = initial relative energy, final relative energy

* EI   EF

   0.   3.

* NS1,NP1,NP3,ND3,ND5,NF5,NF7 = (1) [0] for inclusion (no inclusion)

* of s1/2, p1/2, p3/2, d3/2, d5/2, f5/2, and f7/2 partial waves

* NS   NP1   NP3   ND3   ND5   NF5   NF7

   1   0   0   1   1   0   0

* MP = multipolarity: 0 (M1), 1 (E1), 2 (E2)

* SF = Spectroscopic factor

* MP   SF

   1   1.

* GA = magnetic moment (in units of the nuclear magneton) of

* particle A (core)

* GB = magnetic moment of particle B (proton, neutron, alpha, etc.)

* GA   GB

   -1.7   5.58

****

Only the results for the astrophysical S-factor, S_{17}, for the reaction p+^{8}B will be shown. They are plotted in Figure 4, together with the experimental data of several experiments [25, 26, 28, 29]. The first three set of data (MSU, GSI-1, and GSI-2) were obtained by using the Coulomb dissociation method [30]. The other experimental results [29] were obtained via a direct measurement. The dashed line shows the result of the calculated S-factor, obtained with the bound state wavefunction calculated with the same Woods-Saxon parameters as in the above input file. The dashed line
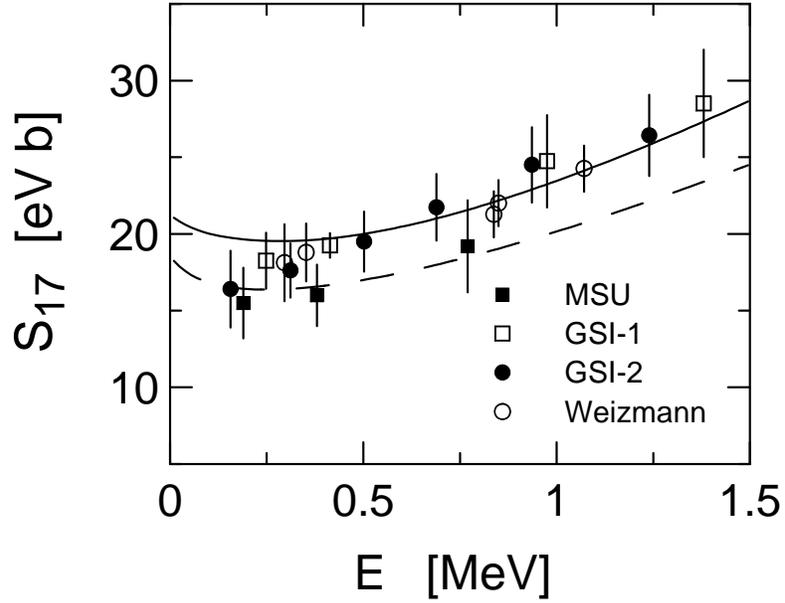
FIG. 4: Astrophysical S-factor for the reaction p+^{8}B. The data are the experimental points of recent experiments [25–29]. The solid and dashed curves are results of calculations with different choices of the Woods-Saxon potential which reproduces the binding of ^{8}B.

represents the S-factor one obtains by changing the bound and continuum states using another set of Woods-Saxon potential parameters, which yields the same binding for ^{8}B, namely:

```
* V0     R0     AA     VS0     RS0     AAS     RC
-30.55   2.95   0.52   -8.53   2.95    0.52    2.95
```

The dashed curve in Figure 4 corresponds to the output file DICAPL.TXT (last column) obtained with the input described above. It is included in the package for checking purposes.

VIII. THINGS TO DO

1 - Use the input files described above and reproduce the Figures 1-4.

2 - Try to reproduce some of the radiative capture cross sections presented in the compilation of Ref. [31].

3 - Show that for neutron halo nuclei the radiative capture cross sections follow the dependence described by equations 42 and 43.

IX. ACKNOWLEDGMENTS

[1] C.E. Rolfs and W. Rodney, "Cauldrons in the Cosmos", Chicago Press, 1988.

[2] R.F. Christy and I. Duck, Nucl. Phys. **24**, 89 (1961).

[3] T.A. Trombello and P.D. Parker, Phys. Rev. **131**, 2582 (1963).

[4] R.G.H. Robertson, Phys. Rev. **C7**, 543 (1973).

[5] G. Bertsch, J. Borysowicz, H. McManus, and W.G. Love, Nucl. Phys. **A284**, 399 (1977).

[6] A.M. Kobos, B.A. Brown, R. Lindsay, and G.R. Satchler, Nucl. Phys. **A425**, 205 (1984).

[7] H. Beer et al., Phys. Rev. **C54**, 2014 (1998).

[8] H. de Vries, C.W. de Jager and C. de Vries, At. Nucl. Data Tables 36, **495**, 536 (1987).

[9] C.J. Joachain, "Quantum Collision Theory", North Holland, 1983.

[10] J. M. Blatt and V. F. Weisskopf, "Theoretical Nuclear Physics", (Wiley & Sons, New York, 1962).

[11] A. Bohr and B. Mottelson, "Nuclear Structure", vol. I (Benjamin, New York, 1969).

[12] A.R. Edmonds, "Angular Momentum in Quantum Mechanics", Princeton University Press, Princeton, 1960.

[13] R.D. Lawson, "Theory of the Nuclear Shell Model", Clarendon Press, Oxford, 1980.

[14] K.H. Kim, M.H. Park, and B.T. Kim, Phys. Rev. **C35**, 363 (1987).

[15] F.C. Barker, Phys. Rev. **C37**, 2920 (1988).

[16] B. A. Brown, A. Etchegoyen, W. D. M. Rae, and N. S. Godwin, Code OXBASH, unpublished.

[17] W.A. Fowler, G.R. Caughlan, and B.A. Zimmerman, Ann. Rev. Astron. Astrophys. **5**, 525 (1967).

[18] C.A. Bertulani and A. Sustich, Phys. Rev. **C46**, 2340 (1992).

[19] T. Otsuka, M. Ishihara, N. Fukunishi, T. Nakamura and M. Yokoyama, Phys. Rev. **C49,** R2289 (1994).

[20] C. Forssén, N.B. Shul'gina, and M.V. Zhukov, Phys. Rev. **C67**, 045801 (2003).

[21] R. G. Breit and E. P. Wigner, Phys. Rev. **49**, 519 (1936).

[22] J.P. Schiffer, Nucl. Phys. **46**, 246 (1963).

[23] P. J. Brussaard and P. W. M. Glaudemans, *Shell Model Applications in Nuclear Spectroscopy*, (North Holland, Amsterdam, 1977).

[24] C. Rolfs and R. E. Azuma, Nucl. Phys. A **227**, 291 (1974).

[25] B. Davids et al., Phys. Rev. Lett. **81**, 2209 (1998); **86**, 2750 (2001).

[26] N. Iwasa et al., Phys. Rev. Lett. **83**, 2910 (1999).

[27] L.T. Baby et al., Phys. Rev. Lett. **90**, 0022501 (2003).

[28] F. Schümann et al., nucl-ex/0304011 (2003).

[29] A.R. Junghans et al., Phys. Rev. Lett. **88**, 41101 (2002).

[30] G. Baur, C.A. Bertulani and H. Rebel, Nucl. Phys. **A458**, 188 (1986).

[31] C. Angulo et al. Nucl. Phys. **A656**, 3 (1999).