Zero-energy determination of the astrophysical S factor and effective-range expansions

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The first three terms of a Taylor expansion of the astrophysical S factor are determined in the potential model of radiative-capture reactions. As input, the radial Schrödinger equation and its inhomogeneous energy derivatives are solved at zero energy. The radial wave function and its energy derivatives are obtained by matching the solutions of these equations with the corresponding exact asymptotic forms. Explicit expressions are derived for the S factor and for its first and second derivatives at zero energy. The same algorithm allows one to accurately determine the first terms of the effective-range expansion. In particular, the effective-range formula converges much faster than the Schwinger-Bethe formula. The method is illustrated with potential-model descriptions of the ${}^3\mathrm{He}(\alpha,\gamma){}^7\mathrm{Be}$, ${}^6\mathrm{Li}(p,\gamma){}^7\mathrm{Be}$, ${}^7\mathrm{Be}(p,\gamma){}^8\mathrm{B}$, and ${}^{16}\mathrm{O}(p,\gamma){}^{17}\mathrm{F}$ reactions.

I. INTRODUCTION

In astrophysics, the determination of reaction rates requires accurate values of radiative-capture cross sections down to very low energies [1,2]. In order to eliminate the main part of the energy dependence of these cross sections, one makes use of the astrophysical S factor defined as

$$S(E) = E \exp(2\pi\eta)\sigma(E), \qquad (1)$$

where E is the energy in the center-of-mass frame, η is the Sommerfeld parameter and σ is the radiative-capture cross section. Except when resonances are present, the behavior of S is in general expected to be rather smooth at low energies. In fact, the astrophysical S factor possesses a Taylor expansion around $E = 0$,

$$S(E) = S(0) + S'(0)E + \tfrac{1}{2}S''(0)E^2 + \cdots. \qquad (2)$$

Restricted to a few terms, this expansion provides an accurate approximation over some energy domain.

Because the energies of interest in astrophysics can usually not be reached experimentally, an extrapolation based on some nuclear model must be performed [3–5]. Extrapolating model results to very low energies and even to zero energy present difficulties which should not be underestimated. Indeed, a model giving accurate numerical results in a large energy domain may fail at energies close to zero because the scattering wave function describing the initial state of the system becomes so small that its numerical determination becomes hazardous. Also, the computation of the Coulomb functions which are necessary to fix the asymptotic normalization may present inaccuracies at very low energies. Recent examples have shown that cases occur where $S(E)$ markedly varies near $E = 0$ making an accurate interpolation difficult [6–8].

Our aim in the present paper is to circumvent the extrapolation problem by performing a direct calculation of the S factor and derivatives at zero energy, i.e., by solving the Schrödinger equation at the single energy $E = 0$. The method is based on a study of the limit of a rescaled scattering wave function and of its derivatives with respect to energy when this energy tends towards zero. These properties being estab-lished, the determination of the Taylor expansion (2) of the S factor becomes very easy. The method will be presented in the framework of the simple potential model (see, for example, Refs. [3–5,9–13]) but its principle can be extended to more sophisticated models. The present algorithm is not aimed at eliminating calculations at higher energies but rather at giving accurate values down to $E = 0$. The philosophy of our method is rather similar to the effective-range expansion in elastic-scattering studies [14–19]. Therefore, it is not surprising that our method will also offer a new algorithm to accurately compute the parameters of this low-energy expansion of the phase shift.

To prevent confusion, let us make two warnings. First our method is not a new way of extrapolating experimental data. It is a new way of obtaining accurate low-energy results in the frame of a well-known model. A similar idea has been exploited in Ref. [13] but only to determine $S(0)$, and in Ref. [7] to derive a Taylor expansion of the S factor for the square-well potential in the extranuclear-capture model [20]. Second, a number of authors loosely use the notations $S(0)$, $S'(0)$, $S''(0)$ for the parameters in a polynomial approximation of the S factor on a given energy domain (see, for example, Ref. [21]). Such a procedure does not provide a Taylor expansion in the mathematical sense which is used in this paper.

In Sec. II, the determination of the coefficients of the S-factor expansion is explained. After defining the notations (Sec. II A) and the basic formulas (Sec. II B), some properties of the Coulomb functions are discussed on the basis of Refs. [22,23] in Sec. II C. Then the algorithm is described and applied to the determination of the S-factor expansion (Sec. II D) and of the effective-range expansion (Sec. II E). Some numerical aspects are discussed in Sec. III. The method is applied to different examples in Sec. IV. Concluding remarks are presented in Sec. V.

II. S-FACTOR EXPANSION AT ZERO ENERGY

A. Definitions and notations

The nuclear Bohr radius is defined as

$$a_N = \hbar^2/\mu Z_1 Z_2 e^2 \qquad (3)$$

and the nuclear Rydberg energy as

$$E_N = \hbar^2/2\mu a_N^2. \tag{4}$$

An important variable at low energies is the squared inverse of the Sommerfeld parameter which reads

$$\frac{1}{\eta^2} = \frac{E}{E_N}. \tag{5}$$

With definitions (3) and (4), the wave number k is given by

$$k^2 = \frac{E}{a_N^2 E_N}. \tag{6}$$

When E tends towards zero, η tends to infinity and the Coulomb wave functions become unpractical. Indeed, the regular function F_l tends to zero while the irregular function G_l tends to infinity. Therefore, we define rescaled Coulomb functions

$$\mathcal{F}_l(E,r) = k^{-1/2} \exp(\pi\eta) F_l(kr) \tag{7}$$

and

$$\mathcal{G}_l(E,r) = \frac{\pi}{2} k^{-1/2} \exp(-\pi\eta) G_l(kr). \tag{8}$$

Their advantage is that they have a finite limit when $E \to 0$. From the properties of the standard Coulomb functions [24], one deduces the Wronskian

$$W\{\mathcal{G}_l, \mathcal{F}_l\} = \pi/2, \tag{9}$$

where $W\{g,f\} = g(df/dr) - f(dg/dr)$. Through Eqs. (7) and (8), we consider the rescaled Coulomb functions as directly depending on the energy E. In the following, we shall use primes to designate derivatives *with respect to energy*. For example, we shall write

$$\mathcal{F}'_l(E,r) = \frac{d}{dE}\mathcal{F}_l(E,r), \quad \mathcal{F}''_l(E,r) = \frac{d^2}{dE^2}\mathcal{F}_l(E,r), \tag{10}$$

and similar expressions for other functions.

B. Potential-model expression of $S(E)$

Let us consider a capture process where two nuclei with respective masses A_1 and A_2 and charge numbers Z_1 and Z_2 fuse into a nucleus with mass A by emitting a photon with wave number k_γ. The energy of the final nucleus with respect to the elastic threshold will be denoted as E_B. Let I_1 and I_2 be the spins of the colliding nuclei and I be the total spin. In the potential model, I is both the channel spin of the scattering wave function and the total intrinsic spin of the final nucleus. Let l_i and l_f be the initial and final orbital angular momenta for the relative motions between the clusters and J_i and J_f be the initial and final total angular momenta resulting from the coupling with the total spin I.

The radiative-capture cross section in the potential model is given for example in Ref. [2]. Here, we prefer to give immediately an expression for the S factor by absorbing the factor $E \exp(2\pi\eta)$ of Eq. (1) into the initial wave function [5,6]. The S factor for an electric transition of multipolarity λ then reads

$$S_{E\lambda}(E) = \tfrac{1}{2}\alpha\hbar c N_{E\lambda} k_\gamma^{2\lambda+1} [I(E)]^2, \tag{11}$$

where α is the fine-structure constant. We shall denote it as $S(E)$ in the following. In practice, this expression is multiplied by a spectroscopic factor for each component of the final state and summed over initial or final angular momenta. Since we are dealing here with low-energy dependences which may vary from one transition to another, we shall neither introduce spectroscopic factors nor perform summations.

In Eq. (11), the normalization factor is given by

$$N_{E\lambda} = 8\pi\left[Z_1\left(\frac{A_2}{A}\right)^\lambda + Z_2\left(-\frac{A_1}{A}\right)^\lambda\right]^2 \frac{(\lambda+1)(2\lambda+1)}{\lambda(2\lambda+1)!!^2} \frac{(2J_i+1)(2J_f+1)(2l_i+1)(2l_f+1)}{(2I_1+1)(2I_2+1)} \begin{pmatrix} l_f & \lambda & l_i \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{Bmatrix} J_f & l_f & I \\ l_i & J_i & \lambda \end{Bmatrix}^2. \tag{12}$$

The photon wave number is related to the initial energy E through

$$k_\gamma = (|E_B| + E)/\hbar c. \tag{13}$$

The matrix element $I(E)$ is given by the one-dimensional integral

$$I(E) = \int_0^\infty u_{l_f}(r) r^\lambda u_{l_i}(E,r) dr, \tag{14}$$

where $u_{l_i}(E,r) \equiv u_{l_i I J_i}(E,r)$ and $u_{l_f}(r) \equiv u_{l_f I J_f}(r)$ are, respectively, the initial and final radial wave functions. These wave functions are eigenfunctions of the Schrödinger equation

$$H_l u_l = E u_l, \tag{15}$$

with respective energies E and E_B. In Eq. (15), the Hamiltonian reads

$$H_l = -\frac{\hbar^2}{2\mu}\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2}\right] + V_N(r) + \tilde{V}_C(r), \quad (16)$$

where μ is the reduced mass of the system, V_N is the nuclear interaction between the clusters, and $\tilde{V}_C(r)$ is the Coulomb interaction between them (for example, a point-sphere Coulomb interaction). The Coulomb interaction between two-point charges will be denoted as V_C in the following. In order to be useful, Eqs. (11) and (14) require a definition of the normalization of u_{l_i} given with the notations (7) and (8) by

$$u_l(E,r) \underset{r\to\infty}{\longrightarrow} \cos\delta_l(E)\mathcal{F}_l(E,r)$$

$$+ \frac{2}{\pi}\exp(2\pi\eta)\sin\delta_l(E)\mathcal{G}_l(E,r). \quad (17)$$

This normalization ensures that u_l has a finite limit when E tends towards zero [5,6]. It will be convenient to make use of a function of the phase shift δ_l defined as

$$D_l(E) = \frac{2}{\pi}[\exp(2\pi\eta) - 1]\tan\delta_l(E), \quad (18)$$

which also has a finite limit when $E\to 0$ (see Sec. II E).

In the following, we concentrate on very low energies, i.e., on energies verifying

$$\exp(-2\pi\eta) \ll 1. \quad (19)$$

This condition is well satisfied for

$$\eta > 1 \quad \text{or} \quad E < E_N. \quad (20)$$

Then, the phase shift δ_l is very small. With notation (18) and approximation (19), the asymptotic form (17) of the radial wave function becomes

$$u_l(E,r) \underset{r\to\infty}{\longrightarrow} \mathcal{F}_l(E,r) + D_l(E)\mathcal{G}_l(E,r), \quad (21)$$

which remains finite at $E=0$.

C. Properties of Coulomb functions

Coulomb functions can be described at low energies on the basis of an expansion in powers of $1/\eta^2$ [22]. Rigorous expressions of such an expansion for F_l and an asymptotic approximation for G_l have been derived by Humblet [23]. Using Eqs. (2.10a) and (4.8a) of Ref. [23], the rescaled functions (7) and (8) can be approximated by

$$\mathcal{F}_l(E,r) = [1-\exp(-2\pi\eta)]^{-1/2}w_l(E)^{1/2}(\pi r)^{1/2}$$

$$\times\left[f_0(x) - \frac{1}{12\eta^2}f_1(x) + \frac{1}{288\eta^4}f_2(x) + O\left(\frac{1}{\eta^6}\right)\right] \quad (22)$$

and

$$\mathcal{G}_l(E,r) = [1-\exp(-2\pi\eta)]^{1/2}w_l(E)^{1/2}(\pi r)^{1/2}$$

$$\times\left[g_0(x) - \frac{1}{12\eta^2}g_1(x) + \frac{1}{288\eta^4}g_2(x) + O\left(\frac{1}{\eta^6}\right)\right] \quad (23)$$

with

$$x = 2(2r/a_N)^{1/2}. \quad (24)$$

The functions $w_l(E)$ [$u_l(\eta)$ in Humblet's notations] read

$$w_l(E) = \prod_{n=1}^{l}\left(1 + \frac{n^2}{\eta^2}\right). \quad (25)$$

Because of Eq. (5), they are polynomials of degree l of the energy. The functions f_i read

$$f_0(x) = I_{2l+1}(x), \quad (26)$$

$$f_1(x) = \left(\frac{x}{2}\right)^2\left[3(l+1)I_{2l+3}(x) + \frac{x}{2}I_{2l+4}(x)\right], \quad (27)$$

$$f_2(x) = \left(\frac{x}{2}\right)^4\left[9(l+1)(l+2)I_{2l+5}(x)\right.$$

$$\left. + 6\left(l+\frac{8}{5}\right)\frac{x}{2}I_{2l+6}(x) + \left(\frac{x}{2}\right)^2 I_{2l+7}(x)\right], \quad (28)$$

while the functions g_i read

$$g_0(x) = K_{2l+1}(x), \quad (29)$$

$$g_1(x) = \left(\frac{x}{2}\right)^2\left[3(l+1)K_{2l+3}(x) - \frac{x}{2}K_{2l+4}(x)\right], \quad (30)$$

$$g_2(x) = \left(\frac{x}{2}\right)^4\left[9(l+1)(l+2)K_{2l+5}(x)\right.$$

$$\left. - 6\left(l+\frac{8}{5}\right)\frac{x}{2}K_{2l+6}(x) + \left(\frac{x}{2}\right)^2 K_{2l+7}(x)\right]. \quad (31)$$

From these expressions, we deduce the limits

$$\mathcal{F}_l^0(r) = \lim_{E\to 0}\mathcal{F}_l(E,r) = (\pi r)^{1/2}f_0(x), \quad (32)$$

$$\mathcal{G}_l^0(r) = \lim_{E\to 0}\mathcal{G}_l(E,r) = (\pi r)^{1/2}g_0(x). \quad (33)$$

Of course, these functions still satisfy the Wronskian relation (9),

$$W\{\mathcal{G}_l^0,\mathcal{F}_l^0\} = \pi/2. \quad (34)$$

The exponential $\exp(-2\pi\eta)$ and all its derivatives tend to zero when E tends to zero. Therefore, the first factor in Eq. (22) or (23) will behave as a constant (i.e., unity) in the calculation of a Taylor expansion and will play no role. Using notations with an upperscript 0 for functions calculated at

zero energy, we can express with Eqs. (22) and (23) the limits of the first derivatives with respect to energy as

$$\mathcal{F}_l'^0(r) = \frac{(\pi r)^{1/2}}{12 E_N}[p_1 f_0(x) - f_1(x)], \qquad (35)$$

$$\mathcal{G}_l'^0(r) = \frac{(\pi r)^{1/2}}{12 E_N}[p_1 g_0(x) - g_1(x)]. \qquad (36)$$

In these expressions, we introduce the constant

$$p_1 = 6 E_N w_l'(0) = 6 \sum_{n=1}^{l} n^2, \qquad (37)$$

which takes the integer value

$$p_1 = l(l+1)(2l+1). \qquad (38)$$

Similarly, the second derivatives with respect to energy of the rescaled Coulomb functions can be written at zero energy as

$$\mathcal{F}_l''^0(r) = \frac{(\pi r)^{1/2}}{(12 E_N)^2}[(p_2 - p_1^2)f_0(x) - 2p_1 f_1(x) + f_2(x)], \qquad (39)$$

$$\mathcal{G}_l''^0(r) = \frac{(\pi r)^{1/2}}{(12 E_N)^2}[(p_2 - p_1^2)g_0(x) - 2p_1 g_1(x) + g_2(x)]. \qquad (40)$$

Here we introduce the constant

$$p_2 = 72 E_N^2 w_l''(0) = 144 \sum_{m>n=1}^{l} m^2 n^2, \qquad (41)$$

which takes the integer value

$$p_2 = \frac{2}{5} l(l^2 - 1)(4l^2 - 1)(5l + 6). \qquad (42)$$

D. Expansion of $S(E)$

Now we have all the ingredients needed to perform a Taylor expansion of the S factor near zero energy. Let us rewrite the expansion (2) restricted to second order as

$$S(E) \approx S(0)(1 + s_1 E + s_2 E^2) \qquad (43)$$

and let us derive computable expressions of the coefficients. From Eqs. (11) and (14), one immediately obtains

$$S(0) = \tfrac{1}{2} \alpha \hbar c N_{E\lambda} (E_B / \hbar c)^{2\lambda + 1} [I(0)]^2, \qquad (44)$$

with the integral

$$I(0) = \int_0^\infty u_{l_f}(r) r^\lambda u_{l_i}^0(r) dr. \qquad (45)$$

A radial wave function $u_l^0(r) \equiv u_l(0, r)$ at zero energy is a solution of the Schrödinger equation

$$H_l u_l^0 = 0. \qquad (46)$$

This solution satisfies the boundary conditions

$$u_l^0(0) = 0 \qquad (47)$$

and

$$u_l^0(r) \underset{r \to \infty}{\to} \mathcal{F}_l^0(r) + D_l(0) \mathcal{G}_l^0(r). \qquad (48)$$

The normalization of the function u_l^0 is fixed by Eq. (48). Using Eq. (34), the normalization condition can also be written as

$$W\{\mathcal{G}_l^0, u_l^0\} \underset{r \to \infty}{\to} \pi/2. \qquad (49)$$

Let $y_0(r)$ be a solution of Eq. (46) satisfying condition (47). The physical solution can be written as

$$u_l^0(r) = c_0 y_0(r), \qquad (50)$$

where the constant c_0 is determined by the asymptotic condition (49). Another Wronskian property of Eq. (48),

$$W\{\mathcal{F}_l^0, u_l^0\} \underset{r \to \infty}{\to} -\frac{\pi}{2} D_l(0), \qquad (51)$$

formally allows calculating $D_l(0)$ from u_l^0. A more efficient method is described in Sec. II E.

The first-order coefficient s_1 in Eq. (43) is obtained by differentiating Eqs. (11) and (14) with respect to E [5,6], yielding

$$s_1 = \frac{S'(0)}{S(0)} = \frac{2\lambda + 1}{E_B} + \frac{2 I'(0)}{I(0)}, \qquad (52)$$

with the energy derivative of the integral given by

$$I'(0) = \int_0^\infty u_{l_f}(r) r^\lambda u_{l_i}'^0(r) dr. \qquad (53)$$

The energy derivative $u_l'^0$ of the radial wave function at zero energy is a solution of the derivative of the Schrödinger equation (15) at the limit $E \to 0$, i.e.,

$$H_l u_l'^0 = u_l^0. \qquad (54)$$

The required solution of this inhomogeneous differential equation verifies

$$u_l'^0(0) = 0. \qquad (55)$$

Its asymptotic form is given by the energy derivative of Eq. (21) at the limit $E \to 0$ as

$$u_l'^0(r) \underset{r \to \infty}{\to} \mathcal{F}_l'^0(r) + D_l(0) \mathcal{G}_l'^0(r) + D_l'(0) \mathcal{G}_l^0(r), \qquad (56)$$

where $\mathcal{F}_l'^0(r)$ and $\mathcal{G}_l'^0(r)$ are given by Eqs. (35) and (36), respectively. In this expression, $D_l'(0)$ is still unknown. Using Eq. (34), one obtains the Wronskian limit

$$W\{\mathcal{G}_l^0, u_l'^0 - \mathcal{F}_l'^0 - D_l(0)\mathcal{G}_l'^0\} \underset{r\to\infty}{\to} 0. \qquad (57)$$

Let $y_1(r)$ be a solution of Eq. (54) with the initial condition (55). This solution may still differ from $u_l'^0(r)$ by an arbitrary solution of the homogeneous Schrödinger equation (46) at zero energy. If we write

$$u_l'^0(r) = y_1(r) + c_1 u_l^0(r), \qquad (58)$$

the unknown constant c_1 can easily be obtained with Eq. (49) from the Wronskian limit (57). Another Wronskian of the asymptotic form (56),

$$W\{\mathcal{F}_l^0, u_l'^0 - \mathcal{F}_l'^0 - D_l(0)\mathcal{G}_l'^0\} \underset{r\to\infty}{\to} -\frac{\pi}{2}D_l'(0), \quad (59)$$

allows, in principle, extracting the value of $D_l'(0)$. As for $D_l(0)$, we shall describe a more efficient method in the next subsection.

The second coefficient s_2 in the Taylor expansion (43) reads

$$s_2 = \frac{S''(0)}{2S(0)} = \frac{\lambda(2\lambda+1)}{E_B^2} + \frac{2(2\lambda+1)}{E_B}\frac{I'(0)}{I(0)} + \frac{I''(0)}{I(0)}$$

$$+ \left[\frac{I'(0)}{I(0)}\right]^2 \qquad (60)$$

with the second energy derivative of the integral given by

$$I''(0) = \int_0^\infty u_{l_f}(r) r^\lambda u_{l_i}''^0(r) dr. \qquad (61)$$

The second derivative $u_l''^0$ can be determined by differentiating Eq. (15) twice and by taking the limit $E\to 0$, i.e.,

$$H_l u_l''^0 = 2u_l'^0, \qquad (62)$$

with the initial condition

$$u_l''^0(0) = 0. \qquad (63)$$

Its asymptotic form is fixed by the second energy derivative of Eq. (21),

$$u_l''^0(r) \underset{r\to\infty}{\to} \mathcal{F}_l''^0(r) + D_l(0)\mathcal{G}_l''^0(r) + 2D_l'(0)\mathcal{G}_l'^0(r)$$

$$+ D_l''(0)\mathcal{G}_l^0(r), \qquad (64)$$

where $\mathcal{F}_l''^0(r)$ and $\mathcal{G}_l''^0(r)$ are given by Eqs. (39) and (40), respectively. Equation (64) leads to the Wronskian property

$$W\{\mathcal{G}_l^0, u_l''^0 - \mathcal{F}_l''^0 - D_l(0)\mathcal{G}_l''^0 - 2D_l'(0)\mathcal{G}_l'^0\} \underset{r\to\infty}{\to} 0 \quad (65)$$

from which the unknown coefficient $D_l''(0)$ disappears. Again a solution of the inhomogeneous equation (62) verifying the boundary condition (63) may contain an arbitrary amount of $u_l^0(r)$. Let $y_2(r)$ be such a solution. The function $u_l''^0$ can be written as

$$u_l''^0(r) = y_2(r) + c_2 u_l^0(r), \qquad (66)$$

where the constant c_2 is determined by imposing condition (65). The Wronskian limit

$$W\{\mathcal{F}_l^0, u_l''^0 - \mathcal{F}_l''^0 - D_l(0)\mathcal{G}_l''^0 - 2D_l'(0)\mathcal{G}_l'^0\}$$

$$\underset{r\to\infty}{\to} -\frac{\pi}{2}D_l''(0) \qquad (67)$$

allows, in principle, extracting the coefficient $D_l''(0)$.

The present algorithm can easily be extended to higher order by solving the inhomogeneous equation

$$H_l u_l^{(n)0} = n u_l^{(n-1)0} \qquad (68)$$

with $u_l^{(n)0}(0) = 0$ and by using its solution $y_n(r) + c_n u_l^0(r)$ to determine the nth energy derivative $u_l^{(n)0}(r)$. The unknown coefficient of the $u_l^0(r)$ component is fixed with the Wronskian limit

$$W\left\{\mathcal{G}_l^0, u_l^{(n)0} - \mathcal{F}_l^{(n)0} - \sum_{j=0}^{n-1}\binom{n}{j}D_l^{(j)}(0)\mathcal{G}_l^{(n-j)0}\right\} \underset{r\to\infty}{\to} 0. \qquad (69)$$

This calculation requires higher terms in the expansions (22) and (23) which can be deduced from Ref. [23]. The value of $D_l^{(n)}(0)$ is formally given by

$$W\left\{\mathcal{F}_l^0, u_l^{(n)0} - \mathcal{F}_l^{(n)0} - \sum_{j=0}^{n-1}\binom{n}{j}D_l^{(j)}(0)\mathcal{G}_l^{(n-j)0}\right\}$$

$$\underset{r\to\infty}{\to} -\frac{\pi}{2}D_l^{(n)}(0). \qquad (70)$$

E. Effective-range expansion

As a byproduct, the present algorithm provides a simple and accurate way of computing the coefficients of the effective-range expansion.

Let us start from the effective-range expansion [14] for an arbitrary partial wave [17–19] given by

$$\frac{2w_l(E)}{a_N}\left[\frac{2}{D_l(E)} + h(\eta)\right] = -\frac{1}{a_l} + \frac{1}{2}r_l k^2 - P_l r_l^3 k^4 + O(k^6), \qquad (71)$$

when notations (18) and (25) are used. The asymptotic expansion of function $h(\eta)$ reads [14,24]

$$h(\eta) = \frac{1}{12\eta^2} + \frac{1}{120\eta^4} + O\left(\frac{1}{\eta^6}\right). \qquad (72)$$

While expression (71) is standard for the s wave, we have modified it a little for other partial waves in order to avoid complicated dimensions for the scattering length a_l, effective range r_l, and shape coefficient P_l [19]. In Eq. (71), a_l and r_l have the dimension of a length for any l and P_l is dimensionless. For $l>0$, the present coefficients differ from other definitions by a factor $l!^2 a_N^{2l}$.

By taking the limit $E \to 0$ of both sides of Eq. (71), one obtains

$$a_l = -\frac{a_N}{4} D_l(0). \tag{73}$$

The scattering length a_l can thus be deduced from the Wronskian limit (51). However, contrary to the Wronskian (49) which is well behaved and can be computed directly, expression (51) is not useful in practice because it involves a difference of two large numbers. Therefore, we rather restart from a more general relation deduced from Eqs. (21) and (9),

$$W\{\mathcal{F}_l, u_l\} \underset{r \to \infty}{\to} -\frac{\pi}{2} D_l(E), \tag{74}$$

which is valid at an arbitrary energy E small enough so that condition (19) is satisfied. If the Wronskian in Eq. (74) is written as an integral expression, one obtains

$$D_l(E) = -\frac{2}{\pi a_N^2 E_N} \int_0^\infty \mathcal{F}_l(E,r) V_{sr}(r) u_l(E,r) dr. \tag{75}$$

The potential $V_{sr}(r)$ appearing in Eq. (75) is the short-range part of the interaction between the colliding nuclei, defined by

$$V_{sr}(r) = V_N(r) + \tilde{V}_C(r) - V_C(r). \tag{76}$$

Notice the difference of Coulomb potentials. Since all the energy-dependent factors have a well-defined limit for $E \to 0$, one obtains

$$D_l(0) = -\frac{2}{\pi a_N^2 E_N} \int_0^\infty \mathcal{F}_l^0(r) V_{sr}(r) u_l^0(r) dr. \tag{77}$$

Equations (73) and (77) provide a simple and accurate way of calculating the scattering length which does not appear in standard textbooks.

Differentiating Eq. (71) leads for $E=0$ to the expression of the effective range

$$r_l = \frac{a_N}{3} \left[1 - p_1 \frac{a_N}{a_l} - \frac{3a_N^2}{2a_l^2} E_N D_l'(0) \right] \tag{78}$$

with p_1 given by Eq. (38). In practice, the effective range r_l cannot be deduced from the Wronskian (59), which is not well behaved. By differentiating Eq. (75), one obtains the accurate integral expression

$$D_l'(0) = -\frac{2}{\pi a_N^2 E_N} \int_0^\infty V_{sr}(r) [\mathcal{F}_l^0(r) u_l'^0(r)$$
$$+ \mathcal{F}_l'^0(r) u_l^0(r)] dr. \tag{79}$$

With Eq. (79), accurate values of the effective range r_l can be deduced from Eq. (78) since the integrand is short ranged. For $l=0$, this approach provides an alternative to the famous Schwinger-Bethe formula [15,16,14], which reads in the present notations

$$r_0 = \frac{16}{\pi a_N D_0(0)^2} \int_0^\infty \{[\mathcal{F}_0^0(r) + D_0(0)\mathcal{G}_0^0(r)]^2 - [u_0^0(r)]^2\} dr. \tag{80}$$

Equation (79) converges much faster than Eq. (80) and remains valid for $l>0$.

The dimensionless shape parameter P_l is given by the second derivative of Eq. (71) as

$$P_l = -\left(\frac{a_N}{2r_l}\right)^3 \left\{ \frac{2}{15} + \frac{1}{18}(4p_1^2 - p_2)\frac{a_N}{a_l} + \frac{2p_1 r_l}{3a_N} \right.$$
$$\left. - \left(\frac{a_N E_N}{a_l}\right)^2 \left[D_l''(0) + \frac{a_N}{2a_l} D_l'(0)^2 \right] \right\}. \tag{81}$$

By differentiating Eq. (75) twice, one obtains the integral expression

$$D_l''(0) = -\frac{2}{\pi a_N^2 E_N} \int_0^\infty V_{sr}(r) [\mathcal{F}_l^0(r) u_l''^0(r) + 2\mathcal{F}_l'^0(r) u_l'^0(r)$$
$$+ \mathcal{F}_l''^0(r) u_l^0(r)] dr, \tag{82}$$

which can be used to accurately determine P_l. In the neutral case for $l=0$, a formula only based on $u_0^0(r)$ is presented in Ref. [25].

The generalization of Eqs. (77), (79), and (82) is obvious.

III. NUMERICAL ASPECTS

The algorithm described in the preceding section can be applied in various ways differing by the numerical technique chosen to solve the differential equations. Here we briefly present our computational choices.

For approximately solving the differential equations, we apply the Numerov algorithm which is valid for inhomogeneous equations as well [26]. A differential equation of the form

$$\frac{d^2 y}{dr^2} = V(r)y + W(r) \tag{83}$$

is discretized as

$$\xi(r+h) = 2\xi(r) - \xi(r-h) + h^2 V(r) y(r)$$
$$+ \frac{1}{12} h^2 [W(r+h) + 10W(r) + W(r-h)], \tag{84}$$

TABLE I. Potential parameters for the radiative-capture reactions (in MeV and fm).

Reaction	l	I	J	V_0	V_{LS}	R	a	R_C
$^3\text{He}(\alpha,\gamma)^7\text{Be}$	0,2			67.67	0	2.477		3.248
	1			85.99	0.922	2.477		3.248
$^6\text{Li}(p,\gamma)^7\text{Be}$	0,2	3/2		51.72	0	2.27	0.65	2.27
	1	3/2	3/2	65.29	0	2.27	0.65	2.27
$^7\text{Be}(p,\gamma)^8\text{B}$ (T)	0,2	2		3.56	0	2.95	0.52	2.95
	1	2		32.62	0	2.95	0.52	2.95
$^7\text{Be}(p,\gamma)^8\text{B}$ (B)	0,2	2		56.18	0	2.39	0.65	2.39
	0,2	1		45.52	0	2.39	0.65	2.39
	1	2	2	46.62	0	2.39	0.65	2.39
$^{16}\text{O}(p,\gamma)^{17}\text{F}$	0			47.212	0	3.553		3.553
	1			36.0	0	3.553		3.553
	2			58.731	0	3.553		3.553

where

$$\xi(r) = y(r)[1 - \tfrac{1}{12}h^2 V(r)]. \tag{85}$$

The initial values are $y(0)=0$ and an arbitrary choice for $y(h)$ [for example, $y(h)=h^l$]. An interesting aspect of the method presented in Sec. II D is that, while c_0 [Eq. (50)], c_1 [Eq. (58)], and c_2 [Eq. (66)] depend on the choices of $y_0(h)$, $y_1(h)$, and $y_2(h)$, the physical quantities $S(0)$, s_1 and s_2 must be almost insensitive to them. This provides an efficient test of the code.

The Wronskian relations (49), (57), and (65) are calculated with a five-point differentiation formula [24]. The value R_1 at which they are calculated must be such that $V_{sr}(R_1)$ be negligible. This is usually realized not far beyond 10 fm. Again the results must be insensitive to the choice of R_1. Using very large values for R_1 (such as the values used for R_2 below) may lead to inaccuracies. The integrals (77), (79), and (82) are accurately computed with a simple constant-step integration from 0 to R_1 [27].

Finally, $I(0)$ and the derivatives $I'(0)$ and $I''(0)$ are also accurately calculated with the same equal-step method but the integration must be extended to a value R_2 which is often much larger than R_1. Values as large as 600 fm are needed in the following. The value obtained in the present method for R_2 is also valid for potential-model calculations at positive energies.

IV. APPLICATIONS

We now illustrate the algorithms described in Sec. II with a few examples. These examples are selected among literature studies of radiative-capture reactions. Two types of potentials are encountered. The Gaussian potentials are written here as $V(r) = -[V_0 + (8V_{LS}/R^2)\boldsymbol{L}\cdot\boldsymbol{S}]\exp(-r^2/R^2)$ and the Woods-Saxon potentials as $V(r) = -V_0\{1 + \exp[(r-R)/a]\}^{-1}$, where V_0, R, and a are parameters. The point-sphere Coulomb potential is used as $\tilde{V}_C$ with a parameter R_C. In all cases, experimental masses are employed [28].

The parameters of the different potentials are summarized in Table I. Woods-Saxon potentials can be distinguished from Gaussian potentials by the occurrence of an entry for a. The potentials are extracted from Ref. [13] for $^3\text{He}(\alpha,\gamma)^7\text{Be}$, from Ref. [11] for $^6\text{Li}(p,\gamma)^7\text{Be}$, and from Refs. [9,12] for $^7\text{Be}(p,\gamma)^8\text{B}$. In the $^3\text{He}(\alpha,\gamma)^7\text{Be}$ case however, we have slightly refitted the published V_0 and V_{LS} for $l=1$ in order to better reproduce the experimental bound-state energies. In the $^6\text{Li}(p,\gamma)^7\text{Be}$ case, we only consider the $I=3/2$ channel spin and neglect the imaginary part of the potential of Ref. [11]. The potentials for $^7\text{Be}(p,\gamma)^8\text{B}$ are denoted as T for Ref. [9] and as B for Ref. [12]. The ^8B binding energy (0.137 MeV) is not accurately reproduced by these potentials (see Table IV) but we did not modify them. The Gaussian potentials for $^{16}\text{O}(p,\gamma)^{17}\text{F}$ are fitted by us.

First, we discuss the effective-range expansion of the $^3\text{He}+\alpha$ system. The zero-energy radial wave function u_0^0 and its energy derivatives $u_0'^0$ and $u_0''^0$ are displayed in Fig. 1. The function u_0^0 exhibits two nodes due to the orthogonality to two bound states of the deep Gaussian potential which simulate Pauli-forbidden states. The derivatives also have nodes. The first one is very close to the first node of u_0^0 but the second one progressively shifts to larger distances. Therefore, the derivatives reach their asymptotic behavior at larger distances than u_0^0. Notice that the relative signs of the derivatives with respect to u_0^0 are significant.

The convergence of Eqs. (73), (78), and (81) is illustrated by Table II. It is very fast for the different coefficients. A comparison between Eq. (78) and the standard approach (80) is also performed. One observes that Eq. (78) provides an accuracy of about 10^{-4} with a step of 0.2 fm, which is not reached with a step of 0.001 fm by Eq. (79). This is not so surprising since Eq. (78) makes use of $u_l'^0$ which brings more physical information about the scattering. The additional effort in calculating $u_l'^0$ seems to be worthwhile. Similarly, we think that our expression for P_0 should be more efficient than generalizations of the expression presented in Ref. [25].

The scattering length, effective range, and shape parameter of the initial partial waves are given in Table III for the different systems. The step h is chosen small enough so that all the displayed digits are converged ($h=0.001$ fm). We give more digits than requested by the physics in order to
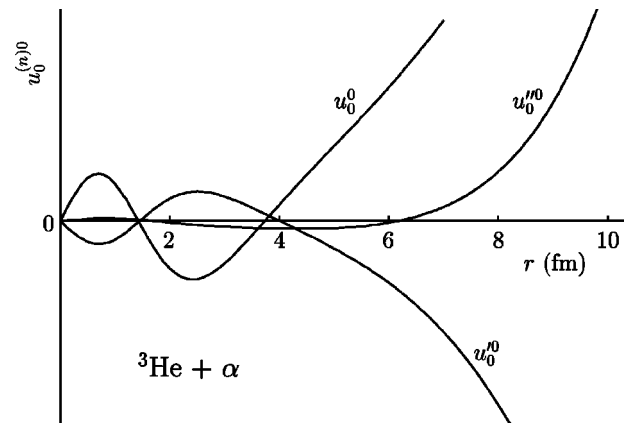

FIG. 1. Zero-energy $^3\text{He}+\alpha$ radial wave function u_0^0 and energy derivatives $u_0'^0$ and $u_0''^0$ in arbitrary units.

TABLE II. Convergence of $l=0$ effective-range coefficients for the ^{3}He$+\alpha$ scattering (h, a_0, and r_0 are in fm).

N	h	a_0	r_0 [Eq. (78)]	r_0 [Eq. (80)]	P_0
24	0.5	36.01899	0.96727	0.5872	-0.091678
60	0.2	36.88286	0.97276	0.7980	-0.090844
120	0.1	36.88984	0.97269	0.8802	-0.090295
240	0.05	36.88732	0.97264	0.9248	-0.090141
600	0.02	36.88631	0.97263	0.9530	-0.090097
1200	0.01	36.88615	0.97263	0.9627	-0.090090
2400	0.005	36.88611	0.97263	0.9677	-0.090089
6000	0.002	36.88610	0.97263	0.9706	-0.090088
12000	0.001	36.88610	0.97263	0.9716	-0.090088

provide a test for the interested reader. In each case, we have checked the effective-range expansion by calculating phase shifts at a number of positive energies.

The s-wave scattering length a_0 is large for the ^{3}He$+\alpha$ and ^{16}O$+p$ systems. It is negative and rather similar for both ^{7}Be$+p$ potentials. The s-wave effective range r_0 is large for ^{6}Li$+p$. The P_0 parameters are often small but the interesting quantity in the effective-range expansion (71) is rather $P_0 r_0^3$ which is large for ^{6}Li$+p$. For $l>0$, the results are not very intuitive but correctly reproduce the phase-shift behaviors. The scattering lengths are often quite small. This is due to the effect of the centrifugal barrier which damps the wave functions in the region where V_{sr} is large in Eq. (77). The corresponding effective ranges are very large because of the occurrence of a_l in the denominators of Eq. (78). They lead to very small shape parameters P_l.

The integrands appearing in the expressions of $I(0)$, $I'(0)$, and $I''(0)$ for the $l_i=0$ component of the ^{3}He$(\alpha,\gamma)^7$Be reaction are displayed in Fig. 2. One observes that the maximum shifts towards larger distances when the order of the derivative increases. The integration must be performed to larger distances R_2 when s_1 and s_2 are calculated than for calculations of $S(0)$ only.

TABLE III. Coefficients of effective-range expansions (a_l and r_l are in fm).

Collision	l	I	a_l	r_l	P_l
^{3}He$+\alpha$	0		36.886	0.9726	-0.09009
	2		2.442×10^{-2}	-900.6	-2.748×10^{-6}
^{6}Li$+p$	0	3/2	1.0228	16.650	0.02165
	2	3/2	-2.693×10^{-4}	2.011×10^{4}	6.258×10^{-10}
^{7}Be$+p$ (T)	0		-4.9966	2.8231	-0.03894
	2		-7.327×10^{-5}	7.639×10^{4}	-8.575×10^{-11}
^{7}Be$+p$ (B)	0	2	-7.8527	4.2455	-0.08322
	2	2	-1.488×10^{-3}	3.138×10^{3}	6.897×10^{-8}
	0	1	2.6088	1.9116	0.4038
	2	1	-1.075×10^{-3}	5.336×10^{3}	2.850×10^{-9}
^{16}O$+p$	0	1/2	6847.9	1.2102	-0.2436
	1	1/2	27.439	-0.4262	47.647
	2	1/2	2.2489	-40.679	-2.197×10^{-3}

The coefficients $S(0)$, s_1, and s_2 in the S-factor expansion (43) are presented in Table IV for selected transitions of the different reactions. The $S(0)$ factors correspond to sums over the possible J_i values in Eq. (12). Summations over l_i, l_f, I, and J_f are not performed here in order to display the energy dependence of each term. To obtain a total S factor, the different l_i contributions must first be added. The results must then be multiplied by spectroscopic factors $\mathcal{S}_{l_f I J_f}$ before performing the other sums. The upper bound R_2 in the integrals varies from 50 fm for ^{6}Li$(p,\gamma)^7$Be and 100 fm for ^{3}He$(\alpha,\gamma)^7$Be to 500 fm for ^{7}Be$(p,\gamma)^8$B and 600 fm for several transitions in ^{16}O$(p,\gamma)^{17}$F. The step h is chosen in such a way that the displayed digits are all significant. This is usually achieved with a step of 0.02 fm. The obtained accuracy is much better than required by the physics of astrophysical applications but should help the reader testing his calculations. Good values can already be obtained with a step of 0.1 fm. Here also, we have checked the expansions with radiative-capture calculations at positive energies.

The s_1 values offer a large variety of situations. Negative values are obtained in most cases for the s and p waves, as is well known from individual studies of these systems. A remarkable exception is the $E2$ capture to the ^{17}F ground state in the ^{16}O$(p,\gamma)^{17}$F reaction. This effect was emphasized and explained in Ref. [8]. In this case, the simple extranuclear-capture model is completely wrong. The very large scattering length implies the existence of a node in the initial wave at large distances, which must be taken into account. As s_2 is even larger, a Taylor expansion is here of little utility. For the d waves, s_1 is positive for all examples and will lead to a slower decrease of the total S factor. The value of s_2 is quite variable.

Let us now compare these results with the literature. In the ^{3}He$(\alpha,\gamma)^7$Be case, our $J_f=3/2$ and $J_f=1/2$ results for $S(0)$ are in good agreement with those of Ref. [13] in spite of a slightly modified final potential.

For the ^{7}Be$(p,\gamma)^8$B reaction, detailed studies have been performed by Barker [12,29] and recently by Jennings, Karataglidis, and Shoppa [7]. Following Ref. [20], Barker determines coefficients $a(=s_1)$ and $b(=2s_2-s_1^2)$ for the total S factor. When we calculate the corresponding quantities
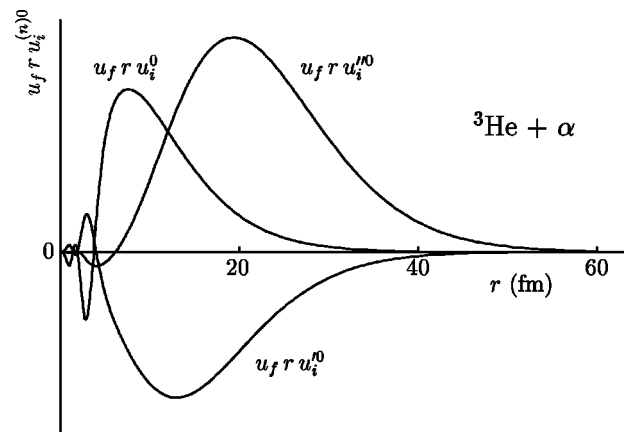

FIG. 2. Integrands of $I(0)$, $I'(0)$, and $I''(0)$ for the $E1$ capture from the s wave of the ^{3}He$(\alpha,\gamma)^7$Be reaction in arbitrary units.

TABLE IV. Coefficients of S-factor expansions (E_B is in MeV and $S(0)$ in MeV b).

Reaction	I	l_i	l_f	J_f	λ	E_B	$S(0)$	s_1	s_2
$^3\mathrm{He}(\alpha,\gamma)^7\mathrm{Be}$	1/2	0	1	3/2	1	-1.5878	3.1803×10^{-4}	-0.8772	0.2586
	1/2	2	1	3/2	1	-1.5878	4.1295×10^{-6}	6.6340	3.9322
	1/2	0	1	1/2	1	-1.1593	1.3785×10^{-4}	-0.9222	0.3797
	1/2	2	1	1/2	1	-1.1593	2.3969×10^{-6}	6.4433	2.8318
$^6\mathrm{Li}(p,\gamma)^7\mathrm{Be}$	3/2	0	1	3/2	1	-5.6143	1.3835×10^{-4}	-0.3277	-0.0338
	3/2	2	1	3/2	1	-5.6143	4.8247×10^{-8}	25.82	104.4
$^7\mathrm{Be}(p,\gamma)^8\mathrm{B}$ (T)	2	0	1	2	1	-0.1161	2.1582×10^{-5}	-2.8350	24.534
	2	2	1	2	1	-0.1161	1.6505×10^{-6}	7.164	-13.216
$^7\mathrm{Be}(p,\gamma)^8\mathrm{B}$ (B)	2	0	1	2	1	-0.1460	2.1762×10^{-5}	-2.2708	15.810
	2	2	1	2	1	-0.1460	1.3363×10^{-6}	8.541	-13.334
	1	0	1	2	1	-0.1460	2.1508×10^{-5}	-2.4143	15.745
	1	2	1	2	1	-0.1460	1.3362×10^{-6}	8.540	-13.353
$^{16}\mathrm{O}(p,\gamma)^{17}\mathrm{F}$	1/2	1	0	1/2	1	-0.1055	1.6532×10^{-2}	-5.5709	45.049
	1/2	1	2	5/2	1	-0.6008	6.1393×10^{-4}	-0.0192	0.2096
	1/2	0	2	5/2	2	-0.6008	6.7548×10^{-8}	44.745	61.495
	1/2	2	0	1/2	2	-0.1055	2.4510×10^{-6}	-0.4377	16.142

with the Barker spectroscopic factors $\mathcal{S}_{122}=0.765$ and $\mathcal{S}_{112} = 0.251$, we cannot reproduce either of the conflicting values in those references. However, our s_2 coefficient is in much better agreement with Ref. [7] than with Ref. [29]. As mentioned in Ref. [7], the numerical determination of a and b (or s_1 and s_2) from $S(E)$ is difficult and must be performed at very low energies (<10 keV in the present case). The large value of s_2, i.e., the strong curvature of $S(E)$, makes this determination especially difficult for the $^7\mathrm{Be}(p,\gamma)^8\mathrm{B}$ reaction. It also indicates that the limited Taylor expansion is valid only at very low energies. For $l=0$, the value of s_1 is in good agreement with the extranuclear-capture result of Ref. [6]. For $l=2$, the values of s_1 and s_2 are almost independent of the potential and very close to the extranuclear-capture estimates.

The $^{16}\mathrm{O}(p,\gamma)^{17}\mathrm{F}$ reaction has been studied in Refs. [6,8]. The s_1 value of the extranuclear-capture model (-5.33 MeV^{-1}) agrees nicely with the present result for the $E1$ capture to the excited state. For the ground-state capture, the small value 0.55 MeV^{-1} is not fully confirmed. Strong curvatures are obtained in Refs. [6,8] for some $E1$ and $E2$ transitions to $^{17}\mathrm{F}$ states in qualitative agreement with the present s_2 values.

V. CONCLUSIONS

The coefficients of the Taylor expansion of the astrophysical S factor can be directly calculated at zero energy. By solving the Schrödinger equation and its energy deriva-tives at $E=0$, one easily obtains the first terms of this expansion. The results are accurate and can be used to check standard calculations at positive energies and to correctly extrapolate them. We think that the present simple technique should become an indispensable complement to future S-factor calculations. However, the Taylor expansion is only valid over a limited energy domain starting at $E=0$ and its coefficients cannot be expected to necessarily provide a good parametrization of the S factor around the Gamow peak.

The method is applied here to the simple potential model but the main ingredients of its algorithm, i.e., the properties of wave functions at zero energy, can straightforwardly be extended to more elaborate models such as the microscopic models [3–5].

In passing, the present approach also offers an alternative way of calculating the coefficients of the effective-range expansion for a given potential. The calculation is based on the same solutions of the Schrödinger equation and its energy derivatives at $E=0$ complemented by simple and fast converging integrals. It is valid for any partial wave. Strikingly, the convergence and accuracy of the effective range are much better than with the traditional Schwinger-Bethe formula.

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