Lagrange mesh calculation of the effective range expansion

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The first terms of the effective range expansion are accurately determined with a small number of evaluations of the potential. The method is based on the *R* matrix theory with a Lagrange basis which leads to a simple meshlike approximation. It is valid for both neutral and charged collisions for arbitrary partial waves. The accuracy of the algorithm is illustrated with an analytically solvable example, with different cases of potential scattering and in particular with the Paris and Bonn nucleon-nucleon potentials.

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I. INTRODUCTION

The insensivity of nucleon-nucleon scattering at low energies to details of the potential has led to the concept of effective range expansion [1–4]. Low-energy phase shifts can be accurately described with two or three parameters: the scattering length, the effective range, and the shape parameter. Initially introduced for the *s* wave, this expansion can be extended to higher partial waves [5,6]. When the colliding particles do not interact through the Coulomb force, the effective range expansion is a truncated Taylor series of a simple function of the phase shift which is analytic as a function of the energy. Such an analytic function also exists when both particles are charged, but is much more complicated. When the determination of the parameters of the effective range expansion is performed with an extrapolation to zero energy, numerical problems may limit their accuracy. For the effective range, this problem is circumvented with the Schwinger-Bethe formula which expresses this quantity with an integral involving the wave function at zero energy. In the absence of Coulomb interaction, the shape parameter is given by a similar formula which involves the energy derivative of the wave function at zero energy [7,8].

Recently, a new algorithm providing a direct calculation of the effective range expansion without extrapolation has been proposed [9]. The parameters are obtained by solving the Schrödinger equation at the single energy $E=0$. The aim of Ref. [9] was to avoid the extrapolation in a calculation of the astrophysical *S* factor and its derivatives at zero energy. It was found that the proposed algorithm simultaneously provided an accurate new technique of determination of the effective range expansion for collisions between charged particles. In particular, the calculation of the effective range is much more accurate than with the Schwinger-Bethe formula. However, the algorithm was mainly aimed at providing the *S* factor expansion and is relatively complicated for the effective range expansion because it requires solving energy derivatives of the Schrödinger equation. Moreover, since the astrophysical problem concerned charged particles, the effective range expansion was determined in that case only.

In the present paper, we propose a new and accurate approach to the calculation of the parameters in the effective range expansion. This method is based on some of the ideas of the algorithm of Ref. [9] but combined with an *R* matrix calculation [10,11] making use of the Lagrange mesh technique [12–14]. In the *R* matrix method, the configuration space is divided into an internal region and an external region at some distance called channel radius. Exact asymptotic expressions of the wave functions are used in the external region. Some convenient basis is used in the internal region. The Lagrange mesh method provides such a basis with the important advantage that the final expressions resemble a mesh calculation [15–18]. The potential matrix is diagonal and only involves values of the potential at the different mesh points. In spite of the extreme simplicity of the method, its accuracy is excellent [12–14]. Here we first extend the *R* matrix theory to zero energy, both in the neutral and charged cases. Then we show how the effective range coefficients can be obtained from the *R* matrix and its energy derivatives at zero energy. With the help of the Lagrange mesh method, their determination is performed without analytical calculation and with only a limited number of evaluations of the potential at the Lagrange mesh points.

Let us emphasize here that, at zero energy, the neutral case is not a limit of the charged case so that rather different treatments are needed. However, as much as possible, we shall try to unify the notations and the presentation in order to take advantage of the fact that the *R* matrix and Lagrange mesh parts of the algorithm are essentially common to both cases.

The simplicity of the present approach partly relies on the analytical knowledge of the limits at zero energy of the solutions of the Schrödinger equation and of their energy derivatives in the external region. The existence of several small corrections to the Coulomb potential (finite size, vacuum polarization, magnetic moment interaction, . . . , see Ref. [19], and references therein) have led to redefinitions of the effective range expansion for nucleon-nucleon scattering [20,21]. The present work provides the ordinary effective range expansion, with no potential or the Coulomb potential in the external region. Long range terms such as the magnetic moment interaction [22] can be handled by choosing a large value for the channel radius.

In Sec. II, the *R* matrix theory on a Lagrange mesh is summarized in a form which can be extended to zero energy. The expressions of the coefficients of the effective range expansion are presented in Sec. III. The method is applied to different examples in Sec. IV. It is shown that it remains very simple even in the presence of the velocity dependent

terms of the Paris and Bonn potentials. Concluding remarks are presented in Sec. V.

II. SUMMARY OF *R* MATRIX THEORY ON A LAGRANGE MESH

The method is described in the single channel case but the extension to several channels is straightforward [14]. Let us consider the potential scattering of two particles with relative coordinate r and reduced mass μ. The configuration space is divided in two regions at an arbitrary channel radius a chosen large enough so that the short-range part of the interaction can be neglected in the external region. In the R matrix method [10,11], the phase shift δ_l of partial wave l at energy $E=\hbar^2k^2/2\mu$ can be expressed as

$$\tan\delta_l(E)=-\frac{F_l(ka)-aR_l(E)dF_l(ka)/da}{G_l(ka)-aR_l(E)dG_l(ka)/da}. \tag{1}$$

In this expression, R_l is the R matrix and F_l and G_l are regular and irregular exact solutions of the asymptotic radial Schrödinger equation employed in the external region.

In the internal region, the dimensionless R matrix can be expressed with N orthonormal basis functions $f_n(r)$ as

$$R_l(E)=\frac{\hbar^2}{2\mu a}\sum_{n,n'=1}^{N} f_n(a)[(C-EI)^{-1}]_{n,n'}f_{n'}(a), \tag{2}$$

where I is the $N\times N$ unit matrix. The matrix C involves the matrix elements

$$C_{nn'}=\int_0^a f_n(r)[T^l+V(r)+\mathcal{L}]f_{n'}(r)dr, \tag{3}$$

where $T^l=-(\hbar^2/2\mu)[d^2/dr^2-l(l+1)/r^2]$ is the kinetic energy operator of partial wave l and V is the potential. The Bloch surface operator [23] is defined as

$$\mathcal{L}=\frac{\hbar^2}{2\mu}\delta(r-a)\frac{d}{dr}. \tag{4}$$

The matrix elements $C_{nn'}$ are obtained very easily when a Lagrange basis is selected.

Let us introduce N functions $f_n(r)$ related to a mesh of N points ax_n defined by

$$P_N(2x_n-1)=0, \tag{5}$$

where $P_N(x)$ is a Legendre polynomial [12,13]. The basis functions $f_n(r)$ and the shifted Legendre mesh satisfy the Lagrange conditions

$$f_{n'}(ax_n)=(a\lambda_n)^{-1/2}\delta_{nn'}. \tag{6}$$

The basis related to shifted Legendre polynomials is expressed as

$$f_n(r)=(-1)^n a^{-1/2}\sqrt{\frac{1-x_n}{x_n}}\,\frac{rP_N[2(r/a)-1]}{r-ax_n}. \tag{7}$$

The coefficients λ_n appearing in Eq. (6) are then given by

$$\lambda_n=[4x_n(1-x_n)]^{-1}[P_N'(2x_n-1)]^{-2}. \tag{8}$$

The x_n and λ_n are easily available since they are nothing but the abscissas and weights of a shifted Gauss-Legendre quadrature [24] in the [0,1] interval

$$\int_0^1 g(x)dx\approx\sum_{n=1}^{N}\lambda_n g(x_n). \tag{9}$$

With the Gauss approximation (9) and the Lagrange condition (6), the kinetic matrix elements read

$$\int_0^a f_n(r)T^l f_{n'}(r)dr\approx T^l_{nn'}=T_{nn'}+\frac{l(l+1)\hbar^2}{2\mu a^2x_n^2}\delta_{nn'}, \tag{10}$$

where the matrix elements $T_{nn'}$ corresponding to the second derivative in T^l are given by $-\lambda_n^{1/2}f_{n'}''(x_n)\hbar^2/2\mu a^2$, i.e.,

$$T_{nn}=\frac{N(N+1)x_n(1-x_n)-3x_n+1}{3x_n^2(1-x_n)^2}\,\frac{\hbar^2}{2\mu a^2}, \tag{11}$$

$$T_{nn'}=(-)^{n+n'+1}\frac{2x_{n'}^2-x_n-x_{n'}}{x_n(x_{n'}-x_n)^2}\sqrt{\frac{x_n(1-x_n)}{x_{n'}(1-x_{n'})^3}}\,\frac{\hbar^2}{2\mu a^2}$$

$$(n'\neq n). \tag{12}$$

The matrix elements of the Bloch operator read

$$\mathcal{L}_{nn'}=\frac{\hbar^2}{2\mu}f_n(a)f_{n'}'(a) \tag{13}$$

with

$$f_n(a)=(-1)^n a^{-1/2}[x_n(1-x_n)]^{-1/2}, \tag{14}$$

$$f_n'(a)=a^{-1}[N^2+N+1-(1-x_n)^{-1}]f_n(a). \tag{15}$$

The sum of $T_{nn'}$ and $\mathcal{L}_{nn'}$ is symmetric. The matrix elements of the potential are calculated approximatively with the Gauss formula (9) which leads to the simple diagonal expression

$$V_{nn'}\approx V(ax_n)\delta_{nn'}. \tag{16}$$

Let us note that the basis (7) is not strictly orthonormal but that we treat it as such because it is orthonormal at the Gauss approximation. Then all expressions appearing in matrix C are very simple.

In order to study limits when E tends towards zero, we have to conveniently choose the definition of the asymptotic solutions. To this end, we renormalize the standard Coulomb functions F_l and G_l. We shall try to treat as much as possible the neutral and charged cases with the same formalism but their low-energy behaviors are completely different. Therefore definitions must be given in a different way in the neutral and charged cases. The renormalized functions $\mathcal{F}_l$

and $\mathcal{G}_l$ will be defined in such a way that their limit at zero energy does not vanish and remains finite [9]. In the neutral case, let us introduce the renormalized spherical Bessel functions

$$\mathcal{F}_l(E,r)=k^{-l}rj_l(kr) \tag{17}$$

and

$$\mathcal{G}_l(E,r)=k^{l+1}rn_l(kr). \tag{18}$$

In the charged case we follow Ref. [9] and define

$$\mathcal{F}_l(E,r)=k^{-1/2}\exp(\pi\eta)F_l(kr) \tag{19}$$

and

$$\mathcal{G}_l(E,r)=\frac{\pi}{2}k^{-1/2}\exp(-\pi\eta)G_l(kr), \tag{20}$$

where η is the Sommerfeld parameter. Equation (1) can now be rewritten as

$$D_l(E)=-\frac{\mathcal{F}_l(E,a)-aR_l(E)\partial\mathcal{F}_l(E,a)/\partial a}{\mathcal{G}_l(E,a)-aR_l(E)\partial\mathcal{G}_l(E,a)/\partial a}. \tag{21}$$

In this expression, D_l has two different meanings, i.e.,

$$D_l(E)=k^{-2l-1}\tan\delta_l(E) \tag{22}$$

in the neutral case and

$$D_l(E)=\frac{2}{\pi}\exp(2\pi\eta)\tan\delta_l(E) \tag{23}$$

in the charged case.

III. EFFECTIVE RANGE EXPANSION

With these notations, the effective range expansion can be written in the neutral case as [4]

$$\frac{1}{D_l(E)}=-\frac{1}{a_l}+\frac{1}{2}r_lk^2-P_lr_l^3k^4+O(k^6). \tag{24}$$

In this expression, a_l is the scattering length, r_l is the effective range, and P_l is the shape parameter of partial wave l. A similar but more complicated expression in the charged case reads [4–6]

$$2\frac{w_l(E)}{l!^2a_N^{2l+1}}\left[\frac{2}{D_l(E)}+h(E)\right]\approx-\frac{1}{a_l}+\frac{1}{2}r_lk^2-P_lr_l^3k^4+O(k^6), \tag{25}$$

where $w_l(E)$ can be expanded as

$$w_l(E)\approx1+\frac{p_1E}{6E_N}+\frac{p_2E^2}{144E_N^2} \tag{26}$$

with $p_1=l(l+1)(2l+1)$ and $p_2=\frac{2}{5}l(l^2-1)(4l^2-1)(5l+6)$, and where $h(E)$ can be approximated by

$$h(E)\approx\frac{E}{12E_N}+\frac{E^2}{120E_N^2}. \tag{27}$$

These expressions involve the nuclear Bohr radius

$$a_N=\hbar^2/\mu Z_1Z_2e^2, \tag{28}$$

where Z_1 and Z_2 are the atomic numbers of the colliding nuclei, and the nuclear Rydberg energy

$$E_N=\hbar^2/2\mu a_N^2. \tag{29}$$

For the s wave, a_0 and r_0 have the dimension of a length and P_0 is dimensionless. For other partial waves, their dimensions are more complicated but identical in the neutral and charged cases. For this reason, we do not follow Ref. [9] where the definitions of the coefficients are modified in the charged case for higher partial waves because the modification would not be applicable to the neutral case.[1]

In the following, we shall use *primes* to designate *derivatives with respect to energy* and *a superscript* 0 to represent *functions at zero energy*. The R matrix and its energy derivatives at zero energy are expressed very simply with Eq. (2). The jth derivative reads

$$R_l^{(j)0}=j!\frac{\hbar^2}{2\mu a}\sum_{n,n'=1}^{N}f_n(a)(C^{-j-1})_{n,n'}f_{n'}(a). \tag{30}$$

The matrix C^{-j-1} is the $(j+1)$th power of the inverse of matrix C and is thus easily obtained.

The energy derivatives of the solutions of the asymptotic equation at zero energy are given in the neutral case by

$$\mathcal{F}_l^{(j)0}(r)=\left(-\frac{\mu}{\hbar^2}\right)^j\frac{r^{l+2j+1}}{(2l+2j+1)!!} \tag{31}$$

and

$$\mathcal{G}_l^{(j)0}(r)=\left(\frac{\mu}{\hbar^2}\right)^j(2l-2j-1)!!r^{-l+2j}. \tag{32}$$

In the charged case, the energy derivatives at zero energy are obtained in Ref. [9] from the properties of Coulomb functions [25,26] as

$$\mathcal{F}_l^0(r)=(\pi r)^{1/2}f_0(x), \tag{33}$$

$$\mathcal{G}_l^0(r)=(\pi r)^{1/2}g_0(x), \tag{34}$$

with

[1]The coefficients a_l, r_l, and P_l of Ref. [9] can be obtained by multiplying the present coefficients by factors $l!^{-2}a_N^{-2l}$, $l!^2a_N^{2l}$, and $l!^{-4}a_N^{-4l}$, respectively.

$$x=2(2r/a_N)^{1/2}. \tag{35}$$

The energy derivatives at zero energy are given by

$$\mathcal{F}_l'^0(r)=\frac{(\pi r)^{1/2}}{12E_N}[p_1 f_0(x)-f_1(x)], \tag{36}$$

$$\mathcal{G}_l'^0(r)=\frac{(\pi r)^{1/2}}{12E_N}[p_1 g_0(x)-g_1(x)], \tag{37}$$

$$\mathcal{F}_l''^0(r)=\frac{(\pi r)^{1/2}}{(12E_N)^2}[(p_2-p_1^2)f_0(x)-2p_1 f_1(x)+f_2(x)], \tag{38}$$

$$\mathcal{G}_l''^0(r)=\frac{(\pi r)^{1/2}}{(12E_N)^2}[(p_2-p_1^2)g_0(x)-2p_1 g_1(x)+g_2(x)]. \tag{39}$$

In these expressions, the functions f_i read

$$f_0(x)=I_{2l+1}(x), \tag{40}$$

$$f_1(x)=\left(\frac{x}{2}\right)^2\left[3(l+1)I_{2l+3}(x)+\frac{x}{2}I_{2l+4}(x)\right], \tag{41}$$

$$f_2(x)=\left(\frac{x}{2}\right)^4\left[9(l+1)(l+2)I_{2l+5}(x)+6\left(l+\frac{8}{5}\right)\frac{x}{2}I_{2l+6}(x)+\left(\frac{x}{2}\right)^2 I_{2l+7}(x)\right], \tag{42}$$

and the functions g_i read

$$g_0(x)=K_{2l+1}(x), \tag{43}$$

$$g_1(x)=\left(\frac{x}{2}\right)^2\left[3(l+1)K_{2l+3}(x)-\frac{x}{2}K_{2l+4}(x)\right], \tag{44}$$

$$g_2(x)=\left(\frac{x}{2}\right)^4\left[9(l+1)(l+2)K_{2l+5}(x)-6\left(l+\frac{8}{5}\right)\frac{x}{2}K_{2l+6}(x)+\left(\frac{x}{2}\right)^2 K_{2l+7}(x)\right], \tag{45}$$

where the functions I_n and K_n are modified Bessel functions [24]. Since expression (21) also involves derivatives with respect to r, one can use in the charged case

$$\frac{d\mathcal{H}}{dr}=\frac{1}{2r}\left(\mathcal{H}+x\frac{\partial\mathcal{H}}{\partial x}\right) \tag{46}$$

for $\mathcal{H}=\mathcal{F}_l^{(j)0}$ and $\mathcal{G}_l^{(j)0}$. From these expressions, the coefficients of the Taylor expansion of $D_l(E)$ can be derived as

$$D_l(0)=-\frac{\mathcal{F}_l^0(a)-aR_l^0 d\mathcal{F}_l^0(a)/da}{\mathcal{G}_l^0(a)-aR_l^0 d\mathcal{G}_l^0(a)/da}, \tag{47}$$

$$D_l'(0)=-\frac{\mathcal{F}_l'^0(a)-aR_l'^0 d\mathcal{F}_l^0(a)/da-aR_l^0 d\mathcal{F}_l'^0(a)/da}{\mathcal{G}_l^0(a)-aR_l^0 d\mathcal{G}_l^0(a)/da}-D_l(0)\frac{\mathcal{G}_l'^0(a)-aR_l'^0 d\mathcal{G}_l^0(a)/da-aR_l^0 d\mathcal{G}_l'^0(a)/da}{\mathcal{G}_l^0(a)-aR_l^0 d\mathcal{G}_l^0(a)/da}, \tag{48}$$

and so on.

The coefficients of the effective range expansion can now be derived. In the neutral case, Eq. (24) leads to the scattering length

$$a_l=-D_l(0). \tag{49}$$

The effective range is given by

$$r_l=-\frac{\hbar^2}{\mu a_l^2}D_l'(0). \tag{50}$$

The shape parameter P_l reads

$$P_l=\frac{a_l}{4r_l}+\frac{1}{8r_l}\left(\frac{\hbar^2}{\mu a_l r_l}\right)^2 D_l''(0). \tag{51}$$

In the charged case, Eqs. (25)–(27) lead to expressions equivalent to those derived in Ref. [9]. The scattering length reads

$$a_l=-\frac{l!^2 a_N^{2l+1}}{4}D_l(0). \tag{52}$$

The effective range is given by

$$r_l=\frac{1}{3l!^2 a_N^{2l-1}}\left[1+\frac{4p_1}{D_l(0)}-\frac{24E_N D_l'(0)}{D_l(0)^2}\right]. \tag{53}$$

The shape parameter P_l reads

TABLE I. Effective range coefficients for the Bargmann potential.

N	a	a_0	r_0	P_0
exact		-23.7654321	2.5974026	0
15	10	-23.7638	2.59734	-5.7×10^{-5}
20	10	-23.7651	2.59732	-5.6×10^{-5}
20	12	-23.76547	2.597397	-5.1×10^{-6}
30	12	-23.765418	2.597398	-5.1×10^{-6}
20	15	-23.764978	2.597409	-3.3×10^{-7}
30	15	-23.7654320	2.5974025	-9.4×10^{-8}

$$P_l=-\frac{1}{36l!^2a_N^{2l-3}r_l^3}\left\{\frac{3}{5}+p_1+\frac{p_2}{D_l(0)}-\frac{24p_1E_ND_l'(0)}{D_l(0)^2}-72E_N^2\left[\frac{D_l''(0)}{D_l(0)^2}-\frac{2D_l'(0)^2}{D_l(0)^3}\right]\right\}. \tag{54}$$

IV. APPLICATIONS

A. Solvable potential

First we test our approach with the solvable Bargmann potential [27] with the conditions of Ref. [28] which simulate neutron-proton scattering when interpreted in fm. The potential reads

$$V(r)=-8b\beta^2\frac{\exp(-2\beta r)}{[1+b\exp(-2\beta r)]^2} \tag{55}$$

with

$$b=\frac{\beta-\alpha}{\beta+\alpha}. \tag{56}$$

Its phase shifts are exactly given by the effective range expansion

$$k\cot\delta=\frac{\alpha\beta}{\beta-\alpha}+\frac{1}{\beta-\alpha}k^2. \tag{57}$$

For $\alpha=0.04$ and $\beta=0.81$, one obtains the results displayed in Table I, which are compared with the exact values. Good results are already obtained with only 15 points for $a=10$. To improve the accuracy, we first increase the number of points for fixed a until the results are stable over the requested digits. Then the radius a is also increased and the procedure is iterated. The accuracy is very high with $N=30$ and $a=15$.

B. Potential scattering

We now illustrate the algorithms described in Sec. II with a few examples. In the neutral case, we consider the ^{9}Li $+n$ system with the potential of Ref. [29] and $\hbar^2/2\mu=(10/9)20.735$ MeV fm^2. It is a Woods-Saxon potential $V(r)=-V_0\{1+\exp[(r-R)/a]\}^{-1}$, with strength $V_0=50.45$ MeV, radius $R=2.642$ fm, and diffuseness $a=0.67$ fm. This potential has a large negative scattering length. This property is believed to be important to explain the halo structure of the ^{11}Li nucleus. As shown in Table II, a reasonable choice for a is 12 fm. Small numbers of points allow one to find accurate values of the different coefficients.

The charged examples have already been studied in Ref. [9] because of their utility for radiative capture reactions. We recalculate their properties here to allow a comparison with the previous approach. Two types of potentials are encoun-

TABLE II. Effective range coefficients for different potentials.

Collision	l	N	a (fm)	a_l(fm^{2l+1})	r_l(fm^{-2l+1})	P_l(fm^{4l})
^{9}Li$+n$	0	20	12	-25.389	7.2207	-0.032392
		30	12	-25.3818	7.2210	-0.032391
		30	14	-25.3835	7.2213	-0.032378
$\alpha+^3$He	0	15	10	36.905	0.97274	-0.09016
		20	10	36.886	0.97260	-0.09007
		30	12	36.885	0.97262	-0.09010
^{7}Be$+p(I=2)$	0	20	12	-7.8521	4.2442	-0.0833
		30	12	-7.8516	4.2444	-0.0833
		30	14	-7.8527	4.2452	-0.0832
^{7}Be$+p(I=1)$	0	20	12	2.6096	1.901	0.4038
		30	12	2.6098	1.901	0.4038
		30	14	2.6090	1.9101	0.4088
^{16}O$+p$	0	30	10	6848	1.2101	-0.2448
		40	10	6850	1.2101	-0.2448
		40	12	6851	1.2102	-0.2437
	1	20	12	402.1	-0.02902	10296
		30	12	402.4	-0.02897	10363
		30	14	402.0	-0.02908	10234

TABLE III. Effective range coefficients for NN potentials.

Potential	NN	$^{2S+1}L_J$	N	a (fm)	a_{LSJ} (fm^{2L+1})	r_{LSJ} (fm^{-2L+1})	P_{LSJ} (fm^{4L})
Minnesota	np	$^1S_0$	15	5	−16.801	2.8849	−0.02864
			20	6	−16.8038	2.88504	−0.02862
		$^3S_1$	15	5	5.42652	1.75766	−0.033118
			20	6	5.42652	1.75766	−0.033118
	pp	$^1S_0$	15	5	−7.8153	2.7223	−0.03154
			20	6	−7.8158	2.7224	−0.03152
Reid	np	$^1S_0$	30	12	−17.137	2.801	0.026
			40	12	−17.139	2.801	0.026
			40	14	−17.144	2.805	0.029
		$^3S_1$	30	12	5.3890	1.7222	−0.0162
			40	12	5.3899	1.7224	−0.0162
			40	14	5.3897	1.7221	−0.0169
	pp	$^1S_0$	30	12	−7.773	2.716	0.033
			40	12	−7.774	2.716	0.033
			40	14	−7.776	2.722	0.037
Paris	np	$^1S_0$	60	12	−17.69	2.876	0.0272
			80	15	−17.702	2.881	0.0312
			80	20	−17.707	2.882	0.0327
		$^3S_1$	50	12	5.4272	1.7636	−0.0045
			60	15	5.4270	1.7634	−0.00532
			60	20	5.4270	1.7635	−0.00524
		$^1P_1$	30	20	2.985	−5.955	−0.00080
			40	25	2.987	−5.979	−0.00063
		$^3P_0$	30	20	−3.056	3.58	−0.022
			40	25	−3.055	3.596	−0.0168
	pp	$^1S_0$	50	12	−7.886	2.79	0.034
			60	15	−7.890	2.802	0.040
			60	20	−7.872	2.807	0.042
		$^3P_0$	30	20	−3.318	3.56	−0.024
			50	25	−3.318	3.583	−0.0178
Bonn	np	$^1S_0$	40	12	−23.74	2.657	0.036
			40	15	−23.749	2.661	0.0399
			50	20	−23.750	2.662	0.0412
		$^3S_1$	40	12	5.4237	1.7590	−0.0048
			40	15	5.4235	1.7587	−0.0057
			50	20	5.4234	1.7589	−0.0057
		$^1P_1$	30	20	3.067	−5.828	−0.0088
			40	25	3.0689	−5.851	−0.0070
		$^3P_0$	30	20	−3.1596	3.104	−0.017
			40	25	−3.1599	3.115	−0.0117
	pp	$^1S_0$	40	12	−8.671	2.593	0.044
			40	15	−8.6746	2.600	0.050
			50	20	−8.6751	2.602	0.0522
		$^3P_0$	30	20	−3.4177	3.132	−0.019
			40	25	−3.4183	3.144	−0.0129

tered: Gaussian potentials and Saxon-Woods potentials, with a point-sphere Coulomb potential. The parameters are given in Table I of Ref. [9]. In all cases, atomic masses [30] are employed. The coefficients of the effective range expansions are displayed in Table II.

For $\alpha+{}^3$He, the Gaussian potential of Ref. [9] is adapted from Ref. [31]. Because of the fast decrease of Gaussian potentials, $a=10$ fm already gives satisfactory results. The last displayed line is in almost perfect agreement with the results of Ref. [9]. However, it is obtained with far less

evaluations of the potential (30 in place of several thousands). In fact, for many practical applications, 20 points would be enough. For $^7\mathrm{Be}+p$, the Woods-Saxon potential is taken from Ref. [32]. Because of the exponential decrease of the potential, the convergence with respect to a is slower, especially for the shape parameter. The agreement with Ref. [9] is excellent for $I=2$ and slightly less good for $I=1$. The Gaussian potentials for $^{16}\mathrm{O}+\mathrm{p}$ are defined in Ref. [9]. For $l=0$, $a=10$ fm already provides good results but this value is too small for $l=1$. The agreement with Ref. [9] is very good if one takes footnote 1 into account in the $l=1$ case. In all cases, 30 or 40 mesh points lead to excellent results.

C. Realistic potentials for nucleon-nucleon scattering

In this section, we consider increasingly sophisticated nucleon-nucleon (NN) interactions. We start with the simple Minnesota central potential which is fitted to the deuteron energy and low-energy scattering properties [33]. The fact that its form factor is a combination of Gaussians makes it popular in resonating group calculations. Then we consider the Reid soft core interaction and its Yukawa form factors [34]. An additional difficulty is introduced by the tensor force which couples some partial waves. Finally we consider the Paris [35] and Bonn [36] realistic interactions. They are less easily tractable because of the occurrence of velocity dependent terms. In all cases, we consider the neutral neutron-proton (np) scattering and the charged proton-proton (pp) scattering.

The results for the Minnesota potential with $\hbar^2/2\mu = 41.47$ MeV fm^2 are displayed in Table III. Because of the use of a common mass for proton and neutron, the np and neutron-neutron (nn) $^1S_0$ cases are identical. Because of the Gaussian decrease of the potential, the small value $a=5$ fm can be selected for the channel radius. Excellent results are obtained with a small number of mesh points ($N=15$). Even the shape parameter displays a fast convergence. Notice that the $^3S_1$ results are more stable and more accurate than the other ones because of the shorter range of the potential in that case. For pp scattering, the same accuracy is obtained as for np $^1S_0$ with the same a and N. In all cases the obtained scattering lengths and effective ranges agree with the values given in Ref. [33].

Accurate results for the Reid potential require a much larger channel radius since the potential decreases exponentially. Hence larger number of mesh points are necessary. The introduction of the tensor potential complicates the calculation for the $^3S_1$ wave because of the coupling with the $^3D_1$ wave. This can easily be solved in the present approach by enlarging the matrix C to both channels in the definition of the single channel R matrix. Good results are already obtained for $a=12$ fm. The convergence of the shape parameter is, however, slower with respect to a. This is related to the increasing spatial extension of the successive derivatives of the wave function with respect to energy (see Fig. 1 of Ref. [9]). Obtaining an accurate shape parameter requires a broader internal region than for the scattering length and the effective range. The results agree well with those of Ref. [34].

The realistic Paris and Bonn potentials contain an additional difficulty with a velocity dependence of the form

$$V(r,p^2)=(p^2/\mu)V^b(r)+V^b(r)(p^2/\mu), \tag{58}$$

where μ is the reduced mass of the NN system [30]. We have treated this term as other terms at the Gauss approximation which leads to the matrix elements

$$\langle V(r,p^2)\rangle_{nn'}\approx 2T^l_{nn'}[V^b(ax_n)+V^b(ax_{n'})]. \tag{59}$$

This approximation preserves the simplicity of the method since it has the same structure as the kinetic energy. Strikingly, it does not significantly reduce the accuracy, although it may slow down convergence.

For the Paris potential, we first use the technique described in Ref. [14] to calculate the deuteron binding energy. With $a=12$ fm and $N=40$, one obtains -2.22472 MeV. When increasing a and N, only the last digit is modified. The coefficients of the effective range are calculated for different partial waves of the np and pp systems. For S waves, the channel radius can be chosen as 15 fm or more. Even larger values are needed for P waves. Larger numbers of mesh points than in the previous cases are needed to get stable results. Nevertheless stable results are obtained with numbers of mesh points of the order of 60 for S waves and 40 for P waves. The convergence of the shape parameter with respect to a is, however, rather slow for the reasons discussed above. Obtaining accurate values for P_{LSJ} requires increasing a and hence N. Our results agree well with those in Table V of Ref. [35]. Notice that our np $^1S_0$ values should be compared with the nn values of that reference in spite of a slight mass difference. The np $^1S_0$ scattering length with this potential is not in good agreement with the experimental one because the potential was fitted on pp scattering.

For the Bonn potential, the deuteron binding energy with $a=12$ fm and $N=40$ is -2.22466 MeV. When increasing a and N, only the last digit is modified. Similar comments as for the Paris potential can be made about the convergence of the results for the effective range expansion. However, one observes that smaller numbers of mesh points are needed for obtaining a given accuracy for the Bonn potential with respect to the Paris potential. This is probably due to the different behaviors of the nonlocal parts. Here the potential is fitted on np scattering and agrees with the experimental np scattering length. The accuracy of the present method allows one to detect small differences between the effective range parameters of the Paris and Bonn potentials for the $^3S_1$ partial wave.

V. CONCLUSIONS

In this paper, we have developed a rather simple algorithm based on the Lagrange mesh technique, which allows an accurate calculation of the coefficients of the effective range expansion. The method of Ref. [9] has been simplified and extended to the neutral case.

The results are obtained without extrapolation and without analytical calculations. They require few evaluations of the potential. Changing from one potential to another is then

very easy. This technique has also been extended to potentials with coupled partial waves and with a velocity dependence, without apparent loss of accuracy.

We have tested the accuracy on a solvable example, on different interesting cases of potential scattering and on different *NN* potentials. Obtaining accurate results requires performing a few calculations with different values of the channel radius and with different number of mesh points. The accuracy is then deduced by keeping the stable digits of the different calculations. Accuracies beyond those requested by physics are easily reached. The velocity dependence of the realistic Paris and Bonn *NN* potentials can be treated without additional complication and without loss of accuracy. The results for these potentials are excellent with numbers of mesh points of the order of 60.

The simplicity of the present approach arises not only from the use of the Lagrange mesh technique but also of the *R* matrix theory. It relies on the existence of known analytical expressions for the asymptotic wave functions. An extension to generalized effective range expansions corresponding to long range terms in the potential is therefore not obvious since these terms modify the wave functions at intermediate distances. This is in particular the case for the small corrections to the Coulomb potential. The coefficients of a generalized effective range expansion might however be obtainable by increasing the channel radius and the number of mesh points. Small deviations from a pure Coulomb behavior might remain within the accuracy of the present method. This problem deserves further study.

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