Equivalence of the Siegert-pseudostate and Lagrange-mesh *R*-matrix methods

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Siegert pseudostates are purely outgoing states at some fixed point expanded over a finite basis. With discretized variables, they provide an accurate description of scattering in the *s* wave for short-range potentials with few basis states. The *R*-matrix method combined with a Lagrange basis, i.e., functions that vanish at all points of a mesh but one, leads to simple meshlike equations which also allow an accurate description of scattering. These methods are shown to be exactly equivalent for any basis size, with or without discretization. The comparison of their assumptions shows how to accurately derive poles of the scattering matrix in the *R*-matrix formalism and suggests how to extend the Siegert-pseudostate method to higher partial waves. The different concepts are illustrated with the Bargmann potential and with the centrifugal potential. A simplification of the *R*-matrix treatment can usefully be extended to the Siegert-pseudostate method.

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I. INTRODUCTION

Recently a new approach for the description of scattering using Siegert pseudostates has been proposed [1,2]. Siegert states are bounded solutions of the Schrödinger equation which are purely outgoing at infinity [3]. These states are particularly interesting because their complex wave numbers provide the poles of the scattering matrix. However, the derivation of these states and their use is not computationally simple. Therefore, Tolstikhin, Ostrovsky, and Nakamura [1,2] have proposed to use modified Siegert states that satisfy purely outgoing conditions at some finite distance. These modified states correspond to exact Siegert states of a truncated potential. The cutoff distance is similar to the channel radius in the *R*-matrix theory and its introduction opens a way to possible relations between the two methods.

The Siegert pseudostates are defined by an expansion of the Siegert states of the truncated potential over a finite basis which becomes complete when the number of basis states tends to infinity. In Refs. [1,2], the authors present an efficient way for deriving the Siegert pseudostates in the *s* wave for short-range potentials. They establish a number of remarkable mathematical properties of these pseudostates and of the corresponding complex wave numbers. This method can be simplified with the help of a Gauss quadrature in the spirit of the discrete-variable representation [4]. Then a simple matrix representation is obtained where the potential matrix is diagonal.

The *R*-matrix theory is a powerful tool, not only to parametrize scattering matrices and cross sections, but also to solve the Schrödinger equation at positive energies [5–7]. In this method, the configuration space is divided into two parts, separated at the channel radius. In the external part, the wave functions are approximated by their asymptotic expressions. In the internal part, a finite basis of square-integrable functions can be used.

The Lagrange-mesh method is an approximate variational calculation which resembles a mesh calculation [8–10]. This property is obtained by using a basis of Lagrange functions, i.e., orthonormal functions that vanish at all points of an associated mesh but one, and the Gauss quadrature corresponding to this mesh. In spite of its simplicity, the accuracy of the Lagrange-mesh method is very high, a property not explained yet [10].

In the single-channel case, Malegat [11] combined the *R*-matrix theory with a Lagrange-mesh method based on shifted Legendre polynomials to study the scattering by a simple solvable potential. Strikingly, the accuracy of the *R*-matrix method on a mesh is as good as the accuracy of the *R*-matrix method using the corresponding Lagrange basis without any approximation [12]. This method can easily be extended to multichannel scattering and gives accurate results for realistic problems [13].

In the present paper, we show that the Siegert-pseudostate method and the *R*-matrix method on a Lagrange mesh are completely equivalent for any basis size when the bases used in both approaches are identical. More strikingly, both methods remain exactly equivalent when their respective mesh approximations are employed. This equivalence sheds light on both approaches. It emphasizes the poorly known fact that the *R*-matrix method can give direct access to the poles of the scattering matrix. The technique presented in Refs. [1,2] provides an accurate practical way of solving this problem for the *s* wave of short-range potentials. Symmetrically, the validity of the *R*-matrix method for higher partial waves and for long-range potentials indicates the way to natural generalizations of the Siegert-pseudostate method.

The *R*-matrix method is summarized in Sec. II. Its application to the Lagrange-Legendre mesh is presented in Sec. III. The equivalence with the Siegert-pseudostate method is discussed in Sec. IV. Examples are commented on in Sec. V. Concluding remarks are presented in Sec. VI.

II. *R*-MATRIX METHOD

As in Ref. [2], we restrict ourselves to a single channel. Contrary to that reference, we first consider an arbitrary partial wave and potentials with a possible Coulomb asymptotic behavior. We follow the notation of Ref. [12]. A translation into the notation of Ref. [2] is delayed to Sec. IV (see also Table I in that section).

For the lth partial wave, the radial Schrödinger equation can be written as

$$(H_l - E)u_l = 0 \tag{1}$$

with $u_l(0)=0$. With $\hbar = m = 1$, the radial Hamiltonian reads

$$H_l = T_l + V(r) = \frac{1}{2}\left(-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} \right) + V(r), \tag{2}$$

where $V(r)$ is a radial potential. The phase shift δ_l is obtained from the asymptotic behavior of bounded solutions

$$u_l(r) \xrightarrow[r\to\infty]{} I_l(kr) - S_l O_l(kr), \tag{3}$$

for positive values of the wave number k corresponding to the energy $E = \frac{1}{2}k^2$. The functions I_l and O_l are ingoing and outgoing Coulomb functions and $S_l = \exp(2i\delta_l)$ is the scattering matrix. In the following k will also take complex values.

In the R-matrix method, the configuration space is divided at the channel radius a into an internal region and an external region. In the external region, the wave function is approximated by its asymptotic form (3). In the internal region, it is expanded on some basis. The formalism is conveniently expressed with the help of the Bloch surface operator [14]

$$\mathcal{L}(B) = \frac{1}{2}\delta(r-a)\left(\frac{d}{dr} - \frac{B}{r} \right), \tag{4}$$

where B is the boundary parameter. The Bloch-Schrödinger equation reads

$$[H_l + \mathcal{L}(B) - E]u_l = \mathcal{L}(B)u_l, \tag{5}$$

where the operator $H_l + \mathcal{L}(B)$ is Hermitian when B is real. The approximation consists in using the asymptotic form (3) in the right-hand side of Eq. (5). The main advantage of the R-matrix method is that an expansion in square-integrable functions can be used in the left-hand side.

Let us consider a set of N basis functions $f_i(r)$ (not necessarily orthogonal) and let us expand u_l in the internal region as

$$u_l(r) = \sum_{j=1}^{N} c_j f_j(r). \tag{6}$$

Equation (5) becomes, after projection on $f_i(r)$,

$$\sum_{j=1}^{N} [C_{ij}(B) - E N_{ij}]c_j = \langle f_i | \mathcal{L}(B) | I_l - S_l O_l \rangle. \tag{7}$$

The elements of the symmetric matrices $\boldsymbol{C}$ and $\boldsymbol{N}$ are defined as

$$C_{ij}(B) = \langle f_i | T_l + \mathcal{L}(B) + V | f_j \rangle = C_{ij}(0) - (B/2a) f_i(a) f_j(a) \tag{8}$$

and

$$N_{ij} = \langle f_i | f_j \rangle. \tag{9}$$

They correspond to one-dimensional integrals over the variable r from 0 to a. Matrix $\boldsymbol{N}$ reduces to the unit matrix when the basis is orthonormal. The right-hand side of Eq. (7) is even simpler. Because of the Bloch operator, it involves values only at $r=a$.

The coefficients c_j are obtained by solving Eq. (7). The continuity condition at $r=a$ between the internal approximation (6) and the asymptotic expression (3) reads

$$\sum_{j=1}^{N} c_j f_j(a) = I_l(ka) - S_l O_l(ka). \tag{10}$$

Let us introduce the external logarithmic derivative L_l at the channel radius,

$$L_l = ka \frac{O_l'(ka)}{O_l(ka)}, \tag{11}$$

and the dimensionless R matrix

$$R_l(B) = (2a)^{-1} \sum_{i,j=1}^{N} f_i(a) [\boldsymbol{C}(B) - E\boldsymbol{N}]^{-1}_{ij} f_j(a). \tag{12}$$

The dependence of the R matrix on the energy E is implied. Introducing c_j in Eq. (10) and using Eqs. (12) and (11), one obtains the scattering matrix for the lth partial wave:

$$S_l = \frac{I_l(ka)}{O_l(ka)} \frac{1 - (L_l^* - B)R_l(B)}{1 - (L_l - B)R_l(B)}, \tag{13}$$

where L_l^* is the conjugate of L_l. Expression (13) has the striking property that it does not depend on the boundary parameter B, independently of the size of the basis. Indeed, from the matrix relation (A4) in the Appendix, one obtains

$$\frac{1}{R_l(0)} = \frac{1}{R_l(B)} + B \tag{14}$$

for any B, real or complex. Introducing relation (14) in Eq. (13) shows that any B value leads to the same scattering matrix as for $B=0$. Equation (14) is well known in R-matrix theory (see Eq. (IV.2.5a) of Ref. [5]). However, its validity for the approximation (12) for any basis size [15] is sometimes overlooked.

The wave function in the internal region is then given by

$$u_l(r) = [2aR_l(B)]^{-1}[I_l(ka) - S_l O_l(ka)] \times \sum_{j=1}^{N} f_j(r) \sum_{i=1}^{N} [\boldsymbol{C}(B) - E\boldsymbol{N}]^{-1}_{ij} f_i(a). \tag{15}$$

Like the scattering matrix S_l and the external wave function $I_l(kr) - S_l O_l(kr)$, this expression does not depend on the choice for B. Indeed, with the help of relation (A3), one easily shows that, for any B, it is equal to the similar expression where B is replaced by zero.

In Refs. [12,13], the parameter B was chosen equal to zero for obvious reasons of simplicity. Another interesting choice is [14,15]

$$B=L_l. \tag{16}$$

This complex value leads to a complex function $R_l(L_l)$ which is not an R matrix in the strict sense since R matrices are real. However, it is also given by expression (12). Equation (13) then takes the simpler form [15]

$$S_l=e^{-2i\phi_l(ka)}[1+2iP_l(ka)R_l(L_l)], \tag{17}$$

where $P_l(ka)$ is defined as

$$P_l=(1/2i)(L_l-L_l^*) \tag{18}$$

and $\phi_l(ka)$ is half the phase of $O_l(ka)/I_l(ka)$. When k is real, P_l is the penetration factor given by the imaginary part of L_l and $\phi_l(ka)$ is the hard-sphere phase shift [5]. Since Eq. (17) has no denominator, a direct relation appears between the poles of the scattering matrix and those of the complex R matrix.

III. *R* MATRIX ON A LAGRANGE MESH

The previous section is valid for arbitrary bases. The calculation of the elements of matrix $\boldsymbol{C}$,

$$C_{ij}(B)=\langle f_i|T_l+\mathcal{L}(0)|f_j\rangle-(B/2a)f_i(a)f_j(a) +\langle f_i|V|f_j\rangle, \tag{19}$$

involves an evaluation of the matrix elements of the potential, which can be tedious and must be repeated when the potential changes. By chosing a Lagrange basis and using the associated Gauss quadrature, one can avoid this calculation without losing accuracy [12].

As Lagrange basis, we use functions based on Legendre polynomials [8,11–13]. These functions are denoted as $\hat{f}_i$ in Ref. [12]. Here as in Ref. [13] we drop the caret because we shall not use any other basis. A Lagrange basis is a set of N functions $f_i(x)$ associated with a Lagrange mesh of N points ax_i on the interval $[0,a]$ [8,9]. The x_i's are zeros of the shifted Legendre polynomial $P_N(2x-1)$ [11], i.e.,

$$P_N(2x_i-1)=0. \tag{20}$$

The Lagrange functions are continuous and indefinitely differentiable anywhere. They read

$$f_i(r)=(-1)^{N-i}a^{-1/2}\sqrt{\frac{1-x_i}{x_i}}\frac{rP_N[2(r/a)-1]}{r-ax_i}. \tag{21}$$

They satisfy the Lagrange conditions

$$f_i(ax_j)=(a\lambda_i)^{-1/2}\delta_{ij}, \tag{22}$$

i.e., each f_i vanishes at all mesh points ax_j, except at ax_i. The coefficients λ_i are the weights associated with a Gauss-Legendre quadrature approximation for the $[0,1]$ interval. The Gauss quadrature on the $[0,a]$ interval reads [16]

$$\int_0^a g(r)dr\approx a\sum_{k=1}^{N}\lambda_k g(ax_k). \tag{23}$$

The weights λ_i are equal to the traditional Gauss-Legendre weights for the $[-1,+1]$ interval, divided by 2.

The Lagrange functions (21) are not orthogonal [12]

$$\langle f_i|f_j\rangle=\delta_{ij}+(-1)^{i+j}\frac{1}{2N+1}\sqrt{\frac{(1-x_i)(1-x_j)}{x_ix_j}}. \tag{24}$$

Because of the Lagrange conditions (22), they are approximately orthogonal at the Gauss approximation (23),

$$\langle f_i|f_j\rangle\overset{\text{Gauss}}{=}\delta_{ij}. \tag{25}$$

Strikingly, using the Gauss approximation does not seem to reduce the accuracy of the R-matrix method [12].

At the Gauss approximation, the potential matrix

$$\langle f_i|V|f_j\rangle\overset{\text{Gauss}}{=}V(ax_i)\delta_{ij} \tag{26}$$

is diagonal because of Eq. (22), and easy to compute. The other matrix elements are *exactly* calculated with the Gauss quadrature. The matrix elements of the sum of the radial part of the kinetic energy and of the Bloch operator are given by

$$\langle f_i|T_0+\mathcal{L}(0)|f_i\rangle=\frac{1}{6a^2x_i(1-x_i)}\times\left[4N(N+1)+3+\frac{1-6x_i}{x_i(1-x_i)}\right] \tag{27}$$

and, for $i\neq j$,

$$\langle f_i|T_0+\mathcal{L}(0)|f_j\rangle=\frac{(-1)^{i+j}}{2a^2[x_ix_j(1-x_i)(1-x_j)]^{1/2}}\times\left[N(N+1)+1+\frac{x_i+x_j-2x_ix_j}{(x_i-x_j)^2}-\frac{1}{1-x_i}-\frac{1}{1-x_j}\right]. \tag{28}$$

Finally, the remaining necessary expressions read

$$\langle f_i|r^{-2}|f_j\rangle=a^{-2}x_i^{-2}\delta_{ij} \tag{29}$$

and

$$\langle f_i|r^{-1}\delta(r-a)|f_j\rangle=a^{-2}(-1)^{i+j}[x_ix_j(1-x_i)(1-x_j)]^{-1/2}. \tag{30}$$

IV. EQUIVALENCE OF THE SIEGERT-PSEUDOSTATE AND *R*-MATRIX METHODS

A. The Siegert-pseudostate method

First we briefly summarize the Siegert-pseudostate method. For this, we keep the R-matrix notation introduced

above. Also, we start with definitions for an arbitrary partial wave. To avoid confusion, the equations of Ref. [2] are denoted as the reference number followed by the equation number in that reference.

The Siegert pseudostates $\phi_l^{(n)}(r)$ with complex wave numbers $k_l^{(n)}$ are solutions of the equation

$$[H_l+\mathcal{L}(L_l^{(n)})-E_l^{(n)}]\phi_l^{(n)}=0, \tag{31}$$

where $L_l^{(n)}$ is calculated for $k=k_l^{(n)}$ and $E_l^{(n)}=\frac{1}{2}k_l^{(n)2}$. Indeed, with the choice $B=L_l$, the right-hand side of Eq. (7) vanishes for purely outgoing waves such as the Siegert pseudostates. For $l=0$ and short-range potentials, definition (31) is exactly equivalent to the pair of equations [2]-(1a) and [2]-(1c′) (see Ref. [14]). Thanks to the use of the Bloch operator, Eq. (31) is more compact.

Expanding $\phi_l^{(n)}$ in the internal region as

$$\phi_l^{(n)}(r)=\sum_{j=1}^{N} c_j^{(n)} f_j(r), \tag{32}$$

one obtains the homogeneous part of Eq. (7),

$$\sum_{j=1}^{N} [C_{ij}(L_l^{(n)})-E_l^{(n)}N_{ij}]c_j^{(n)}=0. \tag{33}$$

However, the dependence of this equation on its eigenvalues $k_l^{(n)}$ is strongly nonlinear because k appears not only in $E=\frac{1}{2}k^2$ but also in L_l.

We now specialize to $l=0$ and short-range potentials. Then the free outgoing wave is given by $O_0=\exp(ikr)$ and the logarithmic derivative reads

$$L_0(ka)=ika. \tag{34}$$

With the help of Eq. (8), the system (33) can be written as

$$\sum_{j=1}^{N}\left[C_{ij}(0)-\frac{1}{2}ik_0^{(n)}f_i(a)f_j(a)-\frac{1}{2}k_0^{(n)2}N_{ij}\right]c_j^{(n)}=0. \tag{35}$$

The eigenvalues $k_0^{(n)}$ appear linearly and quadratically because of the simple form (34) of L_0. Reference [2] provides an efficient algebraic algorithm for solving the system (35), which leads to $2N$ eigenstates. The quadratic matrix eigenvalue problem is replaced by a standard generalized eigenvalue problem of double size. Such a simple algorithm is not yet available for system (33) with $l>0$.

The fact that Eq. (35) can be solved algebraically gives access to the physical poles of the scattering matrix related to the true Siegert states. The other poles obtained are either Siegert states of the truncated potential or nonconverged Siegert states (see the example below). Tolstikhin, Ostrovsky, and Nakamura have shown [Eq. (59) in [2]] that the approximate scattering matrix can then be written as a sum on poles of the form

$$S_0(k)=e^{-2ika}\left[1+ik\sum_{n=1}^{2N}\frac{[\phi_0^{(n)}(a)]^2}{k_0^{(n)}(k_0^{(n)}-k)}\right]. \tag{36}$$

Equivalently, a product expression for the scattering matrix reads [Eq. [2]-(61)]

$$S_0(k)=e^{-2ika}\prod_{n=1}^{2N}\frac{k_0^{(n)}+k}{k_0^{(n)}-k}. \tag{37}$$

This elegant result is valid only for the *s* wave.

The internal wave function ($r\leqslant a$) is given by Eq. [2]-(57), which reads in the present notation

$$u_0(r)=-ike^{-2ika}\sum_{n=1}^{2N}\frac{\phi_0^{(n)}(r)\phi_0^{(n)}(a)}{k_0^{(n)}(k_0^{(n)}-k)}. \tag{38}$$

Equations (36) and (38) assume that the Siegert pseudostates $\phi_0^{(n)}$ are properly normalized [see Eq. [2]-(28)].

B. Equivalence for identical bases

The above equations now allow us to prove the equivalence between the *R*-matrix technique of Refs. [11,12] and the Siegert-pseudostate method of Refs. [1,2]. We shall first show that the approximations giving the scattering matrix are identical for any common finite basis without mesh approximation. To this end, we specialize to $l=0$ and to short-range potentials.

In Refs. [11,12], the boundary parameter B is taken equal to zero but, as proved in Sec. III, exactly the same results would be obtained with any other value. Therefore we now focus on the choice $B=L_0$ with the *s*-wave logarithmic derivative (34). The penetration factor P_0 and the hard-sphere phase shift ϕ_0 take the simple forms

$$P_0(ka)=ka \tag{39}$$

and

$$\phi_0(ka)=ka. \tag{40}$$

Hence, Eq. (17) reads

$$S_0(k)=e^{-2ika}[1+2ikaR_0(ika)]. \tag{41}$$

This expression has the same structure as Eq. [2]-(58), since the R matrix is known to be related to the Green function through

$$R_l=(2a)^{-1}G_l(a,a) \tag{42}$$

[see Eq. (IV.1.10) of Ref. [5]]. It is thus equivalent to Eq. (37) and relates the *S*-matrix and complex *R*-matrix poles.

In order to prove the equivalence of both methods, we have to compare the approximate calculations of these expressions for finite bases. In Ref. [2], the Green function is obtained with Eq. [2]-(49), where the matrix is obtained by inversion from Eq. [2]-(50). Since the matrix appearing in

TABLE I. Symbols of Ref. [2] expressed in the present notation ($l=0$).

Ref. [2]	Equation	Present	Equation
x_i	(C8)	$2x_i-1$	(20)
κ_i	(C11)	$2\lambda_i$	(23)
$\pi_i(x)$	(C9)	$(8a)^{1/2}x_i(x+1)^{-1}f_i[\frac{1}{2}a(x+1)]$	(21)
ρ_{ij}	(C19)	$a^2x_ix_j\langle f_i\|f_j\rangle \equiv a^2x_ix_jN_{ij}$	(24)
$\tilde{K}_{ij}$	(C20)	$a^2x_ix_j\langle f_i\|T_0+\mathcal{L}(0)\|f_j\rangle$	(27),(28)
L_{ij}	(C18)	$\frac{1}{2}a^2x_ix_j\langle f_i\|r^{-1}\delta(r-a)\|f_j\rangle$	(30)
$\tilde{\boldsymbol{H}}+(1-ika)\boldsymbol{L}$	(C15)	$a^2x_ix_j\boldsymbol{C}(ika)$	(19)

Eq. [2]-(50) is identical to the present matrix $\boldsymbol{C}(L_0)-E\boldsymbol{N}$ [see Eq. (8)], the equivalence with our expression (12) is proved.

C. Equivalence of the mesh treatments

We have just shown that, with the same finite basis, both methods are exactly equivalent. Now we show that the same property holds for the discrete-variable-representation (DVR) approximation [4] of Ref. [2] and the Lagrange-mesh approximation of Ref. [12] that is summarized in Sec. III. For $l=0$, both methods make use of a mesh approximation related to zeros of Legendre polynomials.

The R matrix is given by Eq. (12) with matrix $\boldsymbol{C}$ calculated with expression (19) where the different terms can be obtained on the mesh from Eqs. (24) and (26)–(30). In fact the DVR approximation for the Green-function matrix in Ref. [2] is the inverse of a matrix that is proportional to the Lagrange-mesh approximation of matrix $\boldsymbol{C}(ika)-E\boldsymbol{N}$ [Eq. (19)].

The relations between the present quantities and those of Ref. [2] are detailed in Table I. The first line of the table shows that the notation x_i represents different zeros in the two papers: in Ref. [2], they are zeros of a standard Legendre polynomial $P_N(x)$ and belong to $[-1,1]$ while here and in Refs. [11,12] they are zeros of a shifted Legendre polynomial $P_N(2x-1)$ and belong to $[0,1]$. This is only a notational difference. The second line shows the connection between the Gauss weights. The factor of 2 arises from the different lengths of the intervals. The basis functions are related in the third line. The functions $\pi_i(x)$ in Ref. [2] are chosen in such a way that they provide a representation of the unit operator [Eqs. [2]-(5) and [2]-(6)] (see also Ref. [17]). The property [2]-(C13) of these functions shows that they satisfy a Lagrange condition. A compact expression for them has already been derived in Ref. [8] and used in Refs. [11,12] [see the present Eq. (21)]. The present functions $f_i(r)$ may seem to differ by a factor $r=\frac{1}{2}a(x+1)$ but, in Ref. [2], this factor is included in the operator as in Ref. [11]. The overlaps ρ_{ij} differ from the present N_{ij} by a simple factor. Notice that the present form (24) is simpler than expression [2]-(C22) because we do not employ two different bases.

Since the potential matrix elements are approximated in the same way, only the equivalence of the treatments of the kinetic energy remains to be proved. Let us detail the derivation of expressions (27) and (28). Up to a factor 1/2, these matrix elements become with the Gauss quadrature

$$-\int_0^a f_i(r)f_j''(r)dr+\int_0^a f_i(r)\delta(r-a)f_j'(r)dr$$
$$=-(a\lambda_i)^{1/2}f_j''(ax_i)+f_i(a)f_j'(a). \tag{43}$$

The Gauss quadrature is exact for polynomials up to degree $2N-1$ [16] so that expression (43) is exact and leads to Eqs. (27) and (28) (see Ref. [12] for technical details). Equivalently, Eq. (43) can be written as

$$\int_0^a f_i'(r)f_j'(r)dr=a\sum_{k=1}^{N}\lambda_k f_i'(ax_k)f_j'(ax_k). \tag{44}$$

This expression is also exact but less compact. Still another approach is used in Ref. [2]: the left-hand side of Eq. (44) is evaluated analytically after expressing the functions f_i in the basis of Legendre polynomials, in the spirit of the DVR method [4]. The notations for the kinetic-energy matrix elements are compared in the fifth line of Table I. Comparing Eqs. [2]-(C20) and [2]-(C21) for $\tilde{K}_{ij}$ with the present Eqs. (27) and (28) shows that the kinetic-energy matrix elements are calculated much more easily in the Lagrange-mesh philosophy than in the DVR philosophy. We have checked numerically that the expression [2]-(C20) provides exactly the same results as ours, as it should. The notations for the full matrices are compared in the last line of Table I.

Finally, let us mention a difference between the practical applications of the methods of Ref. [2] and of Refs. [11,12]. In Refs. [11,12], expression (24) has been replaced by its Gauss approximation (25): the overlap matrix $\boldsymbol{N}$ is replaced by the unit matrix. This simplification is not used in Ref. [2]. In Ref. [2], the algorithm requires that the equivalent of matrix $\boldsymbol{C}(ika)$ be multiplied to the left and to the right by $\boldsymbol{N}^{-1/2}$. This can easily be done in the present framework (see Sec. V) with $\boldsymbol{N}^{-1/2}$ calculated as explained in the Appendix. However, this complication is useless at the practical level because it does not improve the accuracy [12]. We shall come back to the interest of the simplification (25) when dealing with the first example in Sec. V.

D. Consequences

After these lengthy but necessary technical considerations, let us try to learn some practical consequences from the equivalence of the methods.

For *s* states, the equivalence of the two methods provides a different approach to the determination of the poles of the *S* matrix in the *R*-matrix formalism. Indeed, deriving the complex *S*-matrix poles from the real *R*-matrix poles is not obvious. However the Siegert pseudostates $\phi_l^{(n)}$ appear naturally in the *R*-matrix formalism. They are solutions of Eq. (31) with complex wave numbers $k_l^{(n)}$. For $l=0$, the algebraic algorithm of Ref. [2] provides an efficient way of determining some poles of the *S* matrix with sufficient accuracy. Note that only a few physical poles need usually be determined since the *S* matrix is more conveniently given by Eq. (13) than by Eq. (36) or (37).

Symmetrically the equivalence is also useful to attack the same problem for higher partial waves. The authors of Ref. [2] have tried without success to generalize their search of Siegert pseudostates to $l>0$. They make use of Jacobi polynomials adapted to the value of *l*. This basis was shown in Ref. [12] to be not more efficient than basis (21), but more complicated to use. The reason for this failure is not the technical choice of basis but rather seems rooted in the technique of calculation of the scattering matrix. Indeed, as illustrated later in the second example below, the approximate *wave functions* determined in Ref. [2] should be accurate, up to a normalization factor. As shown at the end of Sec. II, the same approximate wave functions are obtained for any choice of boundary parameter, independently of its physical adequacy. This includes the complex choice (34) which is implicit in Ref. [2]. Hence only the scattering matrix is inaccurate in Ref. [2].

The natural generalization of the Siegert-pseudostate method to $l>0$ and long-range potentials is Eq. (33). However, this equation does not allow one to use the algebraic technique because the nonlinearity is no longer quadratic. We think that it would be useful to use Eq. (33) anyway to derive physical poles of the *S* matrix. The fact that it seems hopeless to find all the pseudostates in this way is of little importance since the *S* matrix can easily and accurately be calculated with the *R*-matrix equation (13). The search for the physical poles could, for example, be performed by extending the iterative algorithm of Descouvemont and Vincke [18].

V. ILLUSTRATIVE EXAMPLES

A. Bargmann potential

Many examples are treated in Ref. [2] and we have reproduced these results. In the case of phase shifts, we have checked that we obtain the same values both with the Siegert-pseudostate method and with the *R*-matrix method within the accuracies of both numerical algorithms. When the number *N* of mesh points is not large enough, both methods provide essentially identical inaccurate results. Rather than repeating here one of those examples, we have chosen a different one which provides interesting intuitive information on the notion of the Siegert pseudostate. We also use this example to discuss more deeply the effect of the Gauss approximation (25) on the overlap matrix element (24).

The Bargmann potential [19,20] is defined as

$$V(r)=-4b^2\beta\frac{e^{-2br}}{(1+\beta e^{-2br})^2} \tag{45}$$

with $\beta=(b-c)/(b+c)$ where *b* and *c* are real parameters. This potential has the remarkable property that its Jost function has only one pole and one zero

$$f_0(k)=\frac{k+ic}{k+ib}. \tag{46}$$

The potential has one bound state for $c<0$ or one virtual state for $c>0$. The scattering matrix reads

$$S_0(k)=\frac{f_0(-k)}{f_0(k)}=\frac{(k+ib)(k-ic)}{(k-ib)(k+ic)}. \tag{47}$$

It possesses the symmetry property $S_0(bc/k)=S_0(k)$. How approximation (37) simulates expression (47) is instructive.

The wave functions of the Siegert states of the potential truncated at *a* read

$$\phi_0^{(n)}(r)\propto\sin k_0^{(n)}r+\frac{b^2-c^2}{k_0^{(n)2}+b^2}\times\frac{k_0^{(n)}\tanh br\cos k_0^{(n)}r-b\sin k_0^{(n)}r}{b+c\tanh br}, \tag{48}$$

where $k_0^{(n)}$ is a solution of the equation

$$\frac{b^2(c+ik)}{\cosh^2 ba}\sin ka=k\left[(b^2+ikc)\tanh^2 ka+b(c+ik)\tanh ba-\frac{k^2+b^2}{b^2-c^2}(b+c\tanh ba)^2\right]\exp(-ika). \tag{49}$$

The unique Siegert state of the Bargmann potential (45) is given by Eq. (48) with the wave number $-ic$, which is an approximate solution of Eq. (49) when *a* is large.

The values $b=2$ and $c=-1$ are selected, which lead to a single bound state at energy $-1/2$. Exact wave numbers of the Bargmann potential truncated at $a=5$, i.e., replaced by zero beyond that value, are displayed as dots in Fig. 1 and in the first two columns of Table II. The isolated wave number close to *i* corresponds to the bound state. It is not exactly *i* because of the finite value of *a*. The pole of the simple Jost function (46) is simulated by a line of wave numbers with imaginary parts close to $-2i$ and rather regularly spaced real parts. The accuracies of the different approximations can be checked with respect to these exact values.

In a first step, we perform a calculation of the wave numbers corresponding to the Siegert pseudostates by following the technique of Ref. [2] without further approximations. For $a=5$ and $N=25$, the values obtained are depicted as circles in Fig. 1. For real parts between about -6.5 and 6.5, they closely correspond to the exact wave numbers of the cutoff Bargmann potential [see panel (a) of Fig. 1]. The remaining

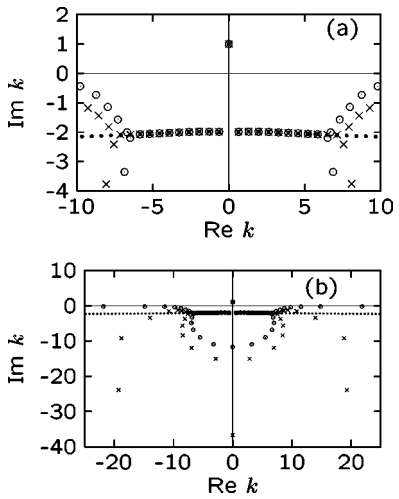

FIG. 1. Complex wave numbers of the Siegert pseudostates of the Bargmann potential: exact (dots); without (circles) and with (crosses) Gauss approximation for the overlap matrix ($a=5$ and $N=25$). Panels (a) and (b) differ only in the scales.

poles split from the exact ones. They do not have any physical significance. They correspond to unconverged solutions of Eq. (35) as shown by the comparison with the exact values in Fig. 1. When N is increased, the horizontal line of physical poles of the cutoff potential obtained with the Siegert-pseudostate method extends to larger values and the nonphysical branches move accordingly.

Numerical values are provided in Table II for $N=25$. The first ones agree within better than 10^{-5} with the exact values. These results are unstable: tiny changes in the computational algorithm (or a change of computer) modify the nonconverged digits. This instability appears to be related to the factors $1-x_i$ in the denominators of expressions (27), (28), and (30), for zeros x_i close to 1. We have also observed that the accuracy in the first wave numbers progressively deteriorates when N becomes larger than 25. This behavior is due to the fact that the norms of the corresponding eigenvectors are very small so that few digits of the eigenvalues are significant. When N increases beyond some value, the number of significant digits of each wave number decreases but the number of physically significant wave numbers nevertheless increases as mentioned above. Because of this important instability of the results for large N, the value $N=25$ is close to optimal for $a=5$ in the present case.

Now we add a simplification to the method by replacing the overlap matrix $\boldsymbol{N}$ by a unit matrix according to the Gauss approximation (25). This approximation has been used in the R-matrix treatment of Refs. [12,13], but it does not introduce much simplification in that case. The algorithm of Ref. [2] is much more simplified by this approximation. The wave numbers obtained are depicted as crosses in Fig. 1. All the physical poles of the cutoff potential remain essentially unmodified (see details in Table II). On the contrary, the structure of the unphysical poles is completely different [see panel (b) of Fig. 1]. As we shall see, this does not affect the phase shift at low energies.

The first values obtained with approximation (25) are essentially identical to those without that approximation (see Table II). This is very surprising because the agreement is much better than the accuracy in these values. When the real part increases, the values become more different, as already illustrated by the figure, but the results obtained with the Gauss approximation first remain better than those obtained with the exact overlap matrix [see panel (a) of Fig. 1]. This effect is also observed in other applications of the Lagrange-mesh method [10].

Phase shifts calculated for different energies with Eq. (37) are displayed in Table III and compared with the exact values from Eq. (47). Because of the symmetry property of the S matrix, the phase shifts at energies E and $b^2c^2/4E$ add to π. The calculations are performed for two choices of channel radius a, i.e., 5 and 6, and for two numbers of mesh points, i.e., 25 and 40.

TABLE II. Complex wave numbers of the Siegert pseudostates of the Bargmann potential: exact [Eq. (49)] and Siegert-pseudostate method without [Eq. (24)] and with [Eq. (25)] the Gauss approximation for the overlap matrix ($a=5$ and $N=25$).

Exact		Equation (24)		Equation (25)	
Re $k_0^{(n)}$	Im $k_0^{(n)}$	Re $k_0^{(n)}$	Im $k_0^{(n)}$	Re $k_0^{(n)}$	Im $k_0^{(n)}$
0	0.9999999999955	0.0000000	0.9999999	0.0000000	0.9999999
0.6390266702	−1.9909403640	0.6390286	−1.9909403	0.6390286	−1.9909403
1.2947020189	−1.9808654900	1.2947061	−1.9808653	1.2947061	−1.9808653
1.9559919327	−1.9824365206	1.9559981	−1.9824363	1.9559981	−1.9824363
2.6142071140	−1.9926145823	2.6142153	−1.9926144	2.6142153	−1.9926144
3.2675033086	−2.0070370919	3.2675133	−2.0070370	3.2675135	−2.0070369
3.9163165163	−2.0231436137	3.9163283	−2.0231433	3.9163285	−2.0231433
4.5614908509	−2.0396289360	4.5615045	−2.0396283	4.5615048	−2.0396285
5.2037975084	−2.0558538335	5.2038193	−2.0558336	5.2038125	−2.0558513
5.8438509338	−2.0715187039	5.8453967	−2.0710367	5.8438594	−2.0715509
6.4821222431	−2.0864975209	6.4948355	−2.1966169	6.4817804	−2.0855307
7.1189698354	−2.1007533271	6.6971747	−2.0045040	7.1321815	−2.0820124
7.7546673954	−2.1142944575	7.2971683	−1.5698719	7.5590343	−2.4165539

TABLE III. Phase shifts (in degrees) of the Bargmann potential: exact [Eq. (47)], Siegert-pseudostate method without [Eq. (24)] and with [Eq. (25)] the Gauss approximation for the overlap matrix, and *R* matrix [Eq. (13)].

E	Exact	a	N	Equation (24)	Equation (25)	Equation (13)
0.1	143.30077480	5	25	143.30076489	143.30076489	143.30076490
			40	143.30076866	143.30076866	143.30076866
		6	25	143.30079803	143.30079803	143.30079803
			40	143.30077472	143.30077472	143.30077473
1	90.00000000	5	25	89.99999083	89.99999083	89.99999083
			40	89.99999947	89.99999947	89.99999958
		6	25	90.00005685	90.00005678	90.00005688
			40	89.99999998	89.99999998	90.00000007
10	36.69922520	5	25	36.69916732	36.69916703	36.69916730
			40	36.69922475	36.69922475	36.69922502
		6	25	36.69975390	36.69974764	36.69974770
			40	36.69922520	36.69922520	36.69922526

For $a=5$ and $N=25$, the relative accuracy in the phase shift is about 10^{-7}, which is better than for the wave numbers. We have also calculated the phase shifts with Eq. (36). The results are inaccurate as mentioned in Ref. [2] because the normalization of the Siegert pseudostates is difficult to achieve numerically: the two terms of the normalization formula [2]-(26) nearly cancel each other for several states. In the following we refer only to Eq. (37). Essentially the same values are obtained with the *R*-matrix mesh method and with both variants of the Siegert-pseudostate method. A difference appears only at $E=10$ but is not significant. The three results are much closer to each other than to the exact one. Increasing the number of mesh points to $N=40$ without modifying a does not really improve the situation at $E=0.1$ but is more useful at higher energies. The remaining disagreement is due to the value of a for which the potential is not yet fully negligible.

For $a=6$ and $N=25$, the relative accuracy in the phase shift is only about 10^{-5}. The number of mesh points is too small for this a value. At all energies, the three approximate results are much closer to each other than to the exact phase shift. When N is increased to 40, the relative accuracy in the phase shifts is better than 10^{-9}. No significant differences between the methods appear. The influence of the approximation (25) is weak for all the energies considered.

B. Purely centrifugal potential

In Ref. [2], the Siegert-pseudostate method is applied to a purely centrifugal potential. In this case, the natural choice (16) for B would be

$$L_1=-1+\frac{(ka)^2}{1-ika}, \tag{50}$$

since $O_1(kr)=-i(1-1/ikr)\exp(ikr)$. The choice $B=L_0=ika$ is made instead in order to use the algebraic algorithm established for $l=0$ short-range potentials. The S matrix is then calculated with Eq. (42) which leads to very inaccurate results as can be expected in the present framework.

The corresponding wave function is, however, essentially independent of the particular choice for B (see Sec. II). Hence, it is as accurate for any nonphysical value of B as for the physical one given by Eq. (50). However, its normalization is not correct. We have verified that the method of Ref. [2], and in particular Eq. [2]-(57) or the present Eq. (38), provides accurate free-particle wave functions for the centrifugal potential, up to a multiplicative factor. This fact seems to have remained unnoticed by the authors of Ref. [2]. It can be understood from the present Eq. (15) to which Eq. (38) is equivalent. Expression (15) is valid for any B but the correct normalization factor $I_l(ka)-S_lO_l(ka)$ is not available to the Siegert-pseudostate method since L_0 is used instead of L_1 and the calculated S matrix is inaccurate. Moreover, this correct scattering wave function is obtained with unphysical Siegert pseudostates and S-matrix poles. These unphysical states are just used as a basis for the expansion of the wave function.

Our result has been obtained with the basis (21) based on Legendre polynomials without recourse to the more complicated Jacobi polynomials employed in Ref. [2]. This confirms the fact established in Ref. [12] that the l-dependent basis of Jacobi polynomials, although accurate, is not necessary to treat $l>0$ partial waves.

VI. CONCLUSIONS

In this paper, we have proved that the Siegert-pseudostate and Lagrange-mesh *R*-matrix methods are in fact exactly equivalent. This property is true when the same finite basis is used in both approaches but also when the mesh methods described in Ref. [2] and in Refs. [12,13] are employed.

This equivalence provides an approximate way of calculating the poles of the S matrix in the *R*-matrix framework for s-wave short-range potentials. It also shows how to generalize the determination of Siegert states for $l>0$ and for long-range potentials but the algebraic algorithm developed in Ref. [2] must be replaced, most probably by some iterative technique.

We have shown that, unexpectedly, the method of Ref. [2] can also be used to construct scattering wave functions for potentials with long-range terms such as the centrifugal term. However, in such cases, the *R*-matrix method of Refs. [12,13] is more advantageous since (i) it is simpler, (ii) it also provides the *S* matrix, and (iii) it is readily extended to the multichannel case.

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APPENDIX

Let $\boldsymbol{B}$ be an invertible matrix and u and v be vectors. The inverse of the matrix

$$\boldsymbol{A}=\boldsymbol{B}+uv^T \tag{A1}$$

is given by

$$\boldsymbol{A}^{-1}=\boldsymbol{B}^{-1}-\frac{\boldsymbol{B}^{-1}uv^T\boldsymbol{B}^{-1}}{1+v^T\boldsymbol{B}^{-1}u}, \tag{A2}$$

where the denominator is a scalar. A corollary of Eq. (A2) reads

$$\boldsymbol{A}^{-1}u=\frac{\boldsymbol{B}^{-1}u}{1+v^T\boldsymbol{B}^{-1}u}. \tag{A3}$$

Another corollary is the relation

$$(v^T\boldsymbol{A}^{-1}u)^{-1}=1+(v^T\boldsymbol{B}^{-1}u)^{-1} \tag{A4}$$

from which Eq. (14) follows.

The norm matrix (24) has the form

$$\boldsymbol{N}=\boldsymbol{1}+\alpha uu^T, \tag{A5}$$

where u is here a unit vector ($\|u\|=1$). Arbitrary powers of $\boldsymbol{N}$ are given by

$$\boldsymbol{N}^\lambda=\boldsymbol{1}+[(1+\alpha)^\lambda-1]uu^T, \tag{A6}$$

for any λ, integer or fractional, positive or negative. In Eq. (24), the components of the unit vector u read

$$u_i=(-1)^i\frac{1}{N}\sqrt{\frac{1-x_i}{x_i}} \tag{A7}$$

and the coefficent α is given by

$$\alpha=N^2/(2N+1). \tag{A8}$$

[1] O.I. Tolstikhin, V.N. Ostrovsky, and H. Nakamura, Phys. Rev. Lett. **79**, 2026 (1997).
[2] O.I. Tolstikhin, V.N. Ostrovsky, and H. Nakamura, Phys. Rev. A **58**, 2077 (1998).
[3] A.J.F. Siegert, Phys. Rev. **56**, 750 (1939).
[4] J.C. Light, I.P. Hamilton, and J.V. Lill, J. Chem. Phys. **82**, 1400 (1985).
[5] A.M. Lane and R.G. Thomas, Rev. Mod. Phys. **30**, 257 (1958).
[6] R.F. Barrett, B.A. Robson, and W. Tobocman, Rev. Mod. Phys. **55**, 155 (1983).
[7] D. Baye and P. Descouvemont, in Proceedings of the 5th International Conference on Clustering Aspects in Nuclear and Subnuclear Systems, Kyoto, Japan, 1988, edited by K. Ikeda, K. Katori, and Y. Suzuki [J. Phys. Soc. Jpn. Suppl. **58**, 103 (1989)].
[8] D. Baye and P.-H. Heenen, J. Phys. A **19**, 2041 (1986).
[9] M. Vincke, L. Malegat, and D. Baye, J. Phys. B **26**, 811 (1993).
[10] D. Baye, M. Hesse, and M. Vincke, Phys. Rev. E **65**, 026701 (2002).
[11] L. Malegat, J. Phys. B **27**, L691 (1994).
[12] D. Baye, M. Hesse, J.-M. Sparenberg, and M. Vincke, J. Phys. B **31**, 3439 (1998).
[13] M. Hesse, J.-M. Sparenberg, F. Van Raemdonck, and D. Baye, Nucl. Phys. A **640**, 37 (1998).
[14] C. Bloch, Nucl. Phys. **4**, 503 (1957).
[15] A.M. Lane and D. Robson, Phys. Rev. **178**, 1715 (1969).
[16] G. Szegö, *Orthogonal Polynomials* (American Mathematical Society, Providence, RI, 1967).
[17] G.W. Wei, J. Phys. B **33**, 343 (2000).
[18] P. Descouvemont and M. Vincke, Phys. Rev. A **42**, 3835 (1990).
[19] V. Bargmann, Rev. Mod. Phys. **21**, 488 (1949).
[20] K. Chadan and P. C. Sabatier, *Inverse Problem in Quantum Scattering Theory* (Springer, New York, 1977).