Jost Function for Coupled Partial Waves

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Abstract

An exact method for direct calculation of the Jost functions and Jost solutions for non-central potentials which couple partial waves of different angular momenta is presented. A combination of the variable-constant method with the complex coordinate rotation is used to replace the matrix Schrödinger equation by an equivalent system of linear first-order differential equations. Solving these equations numerically, the Jost functions can be obtained to any desired accuracy for all complex momenta of physical interest, including the spectral points corresponding to bound and resonant states. The effectiveness of the method is demonstrated using the Reid soft-core and Moscow nucleon–nucleon potentials which involve tensor forces.

I. INTRODUCTION

Almost any textbook on the scattering theory has a chapter devoted to the Jost function, but none of them gives a practical recipe for its calculation; they provide instead equations expressing the Jost function in terms of the wave function. However, to make use of them one must find the wave function first which means that the problem is practically solved and nothing more is needed. Thus one usually gets a feeling that the Jost function is a pure mathematical object, elegant and useful in formal theory, but impractical in computations. This is even more pronounced in problems with non-central potentials which couple partial waves of different angular momenta. To the best of our knowledge, the classical book by Newton [1] is the only one where the coupled partial wave Jost function, which in fact is a matrix–function, is considered and the only calculation of the Jost matrix was done in Ref. [2]. The need of such calculations is of course indisputable since many potentials describing interactions between molecules, atoms, and nuclei are non-central.

It is a widely believed that the Jost function for partial waves coupled by potentials which are non-zero at the origin, is singular and therefore impractical. However, it is not the Jost function but the Jost solution that diverges at $r = 0$. Of course if one wants to obtain the Jost function via the Jost solution, in analogy to un-coupled waves, then the

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problem of singularity is inevitable and thus one must resort to alternative methods.

In this work, we show that the Jost function can be calculated directly by simply solving certain first order coupled differential equations. These equations are based on the variable-phase approach \[^3\] and their solution at any fixed value of the radial variable \( r \), provides the Jost function and its complex conjugate counterpart, which correspond to the potential truncated at the point \( r \). Such equations were proposed in the past for bound and scattering state calculations, that is for calculations in the upper half of the complex momentum plane \[^4\].

Exploiting the idea of the complex rotation of the radial coordinate \[^5\], \( r \to r \exp(i\theta) \), the method was extended to the unphysical sheet so that the resonance state region was also included \[^6\]. This was possible because the coordinate rotation with a sufficiently large \( \theta > 0 \), makes the resonance state wave function quadratically integrable while the energies and widths of the bound and resonance states are not affected since the Jost function and the positions of its zeros do not depend on \( r \). The effectiveness of the method was demonstrated in Ref. \[^7\] for potentials with and without a Coulomb tail where high accuracy for very narrow and very broad resonances was obtained. Its suitability in locating Regge poles in the complex angular momentum plane was also demonstrated. In this paper we generalise the method to non-central potentials that couple different partial waves and show that the complex rotation enables us to calculate the corresponding Jost matrix at all points of the complex momentum plane of physical interest. In a numerical example we demonstrate that a high accuracy can also be achieved.

The paper is organised as follows. In Sec. II and III our formalism is presented, while in Sec. IV the method is applied to several examples and the results obtained are discussed. Our conclusions are given in Sec. V. Finally some mathematical details and proofs are given in the Appendix.

II. FORMALISM

Consider the system of two particles interacting via a non-central potential \( V(\vec{r}) \). Such potentials appear in many physical problems as for example in collisions of elementary and composite particles with non-spherical molecules and in problems involving spin–dependent forces.

Since this type of potentials are not rotationally invariant, the angular momentum \( \ell \) associated with the interparticle coordinate \( \vec{r} \), is not conserved. Therefore a partial–wave decomposition of the Schrödinger equation results in a system of coupled equations for states with different \( \ell \). In general this system consists of an infinite number of equations, and one has to truncate it in order to make it tractable. There are, however, certain problems where only few partial waves are coupled to each other, namely, those in which the non-central part of the potential stems from the nonzero spins of the particles involved. In such systems the total angular momentum,

\[
\vec{J} = \vec{\ell} + \vec{s},
\]
is conserved and the total spin $\vec{s}$ defines the maximal number of coupled partial waves by the triangle condition

$$|J - s| \leq \ell \leq |J + s|.$$  

(1)

In what follows we will consider a problem of this kind though all formulae remain applicable to the more general case of coupled partial waves.

**A. Partial waves for discrete spectrum**

Wave functions $\Psi_{kJM}(\vec{r})$ describing bound and Siegert (resonance) states are specified by a definite value of the momentum $k$, the total angular momentum $J$ and its third component $M$, and the parity $\pi$ which is omitted in our notation. Such wave functions can be expanded in terms of the spin–angular functions

$$\mathcal{Y}_{\ell s}^{JM}(\hat{r}) \equiv \sum_{m\mu} C_{\ell ms\mu}^{JM} Y_{\ell m}(\hat{r}) \chi_{s\mu},$$

as

$$\Psi_{kJM}(\vec{r}) = \frac{1}{r} \sum_{[\ell]} \mathcal{Y}_{\ell s}^{JM}(\hat{r}) u_{[\ell]}^J(k, r),$$

(2)

where $u_{[\ell]}^J(k, r)$ are unknown radial functions, and $[\ell]$ stands for the pair of subscripts $ls$. This notation has the advantage that all formulae remain the same for non–central interactions of spinless particles in which case the symbol $[\ell]$ stands for another pair of quantum numbers, namely, $\ell m$ instead of $ls$. Furthermore all formulae can be generalised to coupled hyperradial equations simply by replacing $[\ell]$ by $[L]$ where $L$ is the grand orbital quantum number (for hyperradial equations see Ref. [8]). In what follows we drop, for simplicity, the quantum numbers $JM$ where this does not cause a misunderstanding.

Substituting the expansion (2) into the Schrödinger equation, one arrives at the following system of coupled equations

$$\left[ \partial_r^2 + k^2 - \ell(\ell + 1)/r^2 \right] u_{[\ell]}^J(k, r) = \sum_{[\ell']} W_{[\ell][\ell']}^J(r) u_{[\ell']}^J(k, r),$$

(3)

where the index $[\ell]$ runs over all combinations of $\ell$ and $s$ allowed by the triangle condition (1) and the parity conservation law. The elements of the matrix $W$ are those of the operator $V(\vec{r})$ (we use $\hbar=1$),

$$W_{[\ell][\ell']}^J(r) \equiv 2m \left\langle \mathcal{Y}_{[\ell]}^{JM} \right| V(\vec{r}) \left| \mathcal{Y}_{[\ell']}^{JM} \right\rangle,$$

(4)

sandwiched between the spin–angular functions (m is the reduced mass). We assume that these matrix elements are less singular at the origin than the centrifugal term,

$$\lim_{r \to 0} r^2 W_{[\ell][\ell']}^J(r) = 0,$$

(5)

and vanish at large distances faster than the Coulomb potential,

$$\lim_{r \to \infty} r W_{[\ell][\ell']}^J(r) = 0.$$
B. Partial waves for continuum

The scattering state wave function $\Psi_{\vec{k}_s\mu}(\vec{r})$ is defined by the real vector $\vec{k}$ (the momentum of the incoming wave), total spin $s$, and its third component $\mu$. The partial wave decomposition for this function is more complicated than for the bound and Siegert states because the scattering state depends on the direction of the incident momentum $\vec{k}$. Since $\Psi_{\vec{k}_s\mu}(\vec{r})$ depends on the two vectors $\vec{k}$ and $\vec{r}$, we have to perform partial wave analysis in both the momentum and coordinate space [1,9],

$$\Psi_{\vec{k}_s\mu}(\vec{r}) = \sqrt{\frac{2}{\pi k r}} \sum_{JM[\ell]J'su} Y_{J'M}^{JM}(\hat{r}) u_{[\ell][s]}^{J'}(k, r) Y_{[\ell]'\mu}^{J'M*}(\hat{k}),$$  \hspace{1cm} (7)

where

$$Y_{[\ell][s]}^{JM}(\hat{k}) \equiv i^{-\ell} \sum_{m} C_{[\ell][s]m}^{JM} Y_{[\ell]m}(\hat{k}),$$

and the radial wave function $u_{[\ell][s]}^{J'}(k, r)$ obeys the same equation as $u_{[\ell]}(k, r)$,

$$\left[ \partial_r^2 + k^2 - \ell(\ell + 1)/r^2 \right] u_{[\ell][s]}^{J'}(k, r) = \sum_{[\ell']}[\ell'] W_{[\ell][\ell']}^{J'}(r) u_{[\ell']}^{J'}(k, r).$$  \hspace{1cm} (8)

Physical solutions of Eqs. (3) and (8) are defined by the requirement that they must be regular at the origin,

$$u_{[\ell]}(k, r) \rightarrow 0 \quad r \rightarrow 0,$$

$$u_{[\ell][s]}^{J'}(k, r) \rightarrow 0 \quad r \rightarrow 0,$$  \hspace{1cm} (9)

and by certain, physically motivated, boundary conditions at infinity,

$$u_{[\ell]}(k, r) \rightarrow U_{[\ell]}(k, r) \quad r \rightarrow \infty,$$

$$u_{[\ell][s]}^{J'}(k, r) \rightarrow U_{[\ell][s]}^{J'}(k, r),$$  \hspace{1cm} (10)

which are different for the various problems (bound, scattering, and resonant states) and change drastically when we go over from one case to another. It would be, of course, more convenient to deal with a universal boundary conditions imposed at a single point. This can be achieved if we consider the general regular solution of Eq. (8) defined only by the condition (9) and not subjected to any restrictions at large $r$. This is described next.

C. Regular basis

From the vast variety of solutions obeying (8) and having different behaviour at large distances we choose only those which are linearly independent. They form the fundamental system of regular solutions which we call regular basis. Any regular solution with a specific behaviour at large distances, is simply a linear combination of the basic solutions. Thus,
instead of having different mathematical procedures for the various types of physical problems we can have only one for the regular basis. In the next section we show how the bound, scattering, and resonant state wave functions can be constructed in terms of such a basis.

Let us consider Eq. (3) as a matrix equation. Then, each of its solutions is a column–matrix. From the general theory of differential equations is known that there are as many independent regular column–solutions of Eq. (3) as the column dimension, i.e., the number of equations in the system. These columns can be combined in a square matrix \( \Phi \) satisfying

\[
\left[ \partial^2_r + k^2 - \ell(\ell + 1)/r^2 \right] \Phi_{[\ell][\ell']} (k, r) = \sum_{[\ell'']} W_{[\ell][\ell'']} (r) \Phi_{[\ell''][\ell']} (k, r),
\]

(11)

with

\[
\Phi_{[\ell][\ell']} (k, r) \to 0, \quad \forall \ [\ell], [\ell'].
\]

(12)

Since Eq. (11) is of second order and singular at \( r = 0 \), the condition (12) cannot be reduced to the simple requirement

\[
\Phi_{[\ell][\ell']} (k, 0) = 0, \quad \forall \ [\ell], [\ell'],
\]

as the behaviour of each element of the matrix \( \Phi(k, r) \) and its first derivative \( \partial_r \Phi(k, r) \) in the immediate vicinity of the point \( r = 0 \) are also needed.

Like in any other space, the basis can be chosen in an infinite number of ways by specifying the behaviour (12). The possible choice of the condition (12), however, is not entirely arbitrary. It was shown in Ref. [10] (see also an alternative proof in the Appendix) that for potentials fulfilling the restriction (5), the regular columns are linearly independent only if they vanish near the point \( r = 0 \) in such a way that

\[
\lim_{r \to 0} \frac{\Phi_{[\ell][\ell']} (k, r)}{r^{\ell' + 1}} = \delta_{[\ell][\ell']}. \tag{13}
\]

The primed angular momentum in the denominator means that in each row of the matrix \( \|\Phi_{[\ell][\ell']}\| \) the elements, situated further to the right, vanish faster when \( r \to 0 \). Even without a formal proof it is clear that such condition guarantees the linear independence of the columns since in each row the elements have different behaviour (different power of \( r \)) near \( r = 0 \). If instead of the rows, we look at the columns, we get from Eq. (13) that in each of them all off-diagonal elements are infinitesimal as compared to the diagonal one.

Yet in spite of the restriction (13), we still have some freedom in specifying the derivatives \( \partial_r \Phi_{[\ell][\ell']} \). Indeed, we can choose at least an arbitrary \( r \)–independent coefficient in each element of the matrix \( \|\Phi_{[\ell][\ell']}\| \). We mention here that it was this freedom which was exploited by Newton in his procedure of regularisation of the integral equation for \( \Phi_{[\ell][\ell']} \).

To be consistent with the definition of the regular solution for the un-coupled partial waves [11], we choose the normalisation coefficients in such a way that
where \( j_\ell(z) \) is the Riccati–Bessel function \([12]\). This condition defines the leading terms of the near–origin behaviour of the diagonal elements of the matrix \( \|\Phi_{[\ell][\ell']}\| \) and their first derivatives. The off-diagonal elements, however, remain obscure since the condition \([14]\) only implies that \( \Phi_{[\ell][\ell']} \sim o(j_\ell), \ell \neq \ell' \). As pointed out by Newton \([1]\), it is impossible to define them unambiguously by boundary conditions which are independent of the behaviour of the potential near the origin. In the Appendix we show that this is indeed the case and we give a simple recipe for obtaining series expansions of all matrix elements of \( \|\Phi(k, r)\| \) at \( r \sim 0 \). Of course, the terms of such series depend also on the potential.

In principle, from the knowledge of such expansions, we could calculate the matrix \( \|\Phi(k, r)\| \) by solving the Schrödinger equation \([11]\) directly. It is, however, much more convenient to transform Eq. \([11]\) into another equivalent form suitable for a construction of different physical solutions. For this we introduce two new unknown matrices \( \|F_{[\ell][\ell']}^{(\pm)}(k, r)\| \) and assume the following ansatz for the regular solution

\[
\Phi_{[\ell][\ell']}^{(\pm)}(k, r) = \frac{1}{2} \left[ h_\ell^{(+)}(kr)F_{[\ell][\ell']}^{(+)}(k, r) + h_\ell^{(-)}(kr)F_{[\ell][\ell']}^{(-)}(k, r) \right]
\]

where the Riccati–Hankel functions \( h_\ell^{(\pm)} \) are linear combinations of the Riccati–Bessel and Riccati–Neumann functions \( h_\ell^{(\pm)}(z) = j_\ell(z) \pm in_\ell(z) \) \([12]\). The reason for choosing such an ansatz will become clear in the next section. Here it is sufficient to say that the explicit implantation of the functions \( h_\ell^{(\pm)}(kr) \) into the construction of the basis guarantees the correct asymptotic behaviour of the basic solutions at large \( r \).

Since instead of one unknown matrix \( \|\Phi\| \) we introduced two matrices \( \|F^{(\pm)}\| \), they must be subjected to an additional constrain. The most convenient is the Lagrange condition

\[
h_\ell^{(+)}(kr)\partial_r F_{[\ell][\ell']}^{(+)}(k, r) + h_\ell^{(-)}(kr)\partial_r F_{[\ell][\ell']}^{(-)}(k, r) = 0,
\]

which is a standard choice in the variable–constant method for solving differential equations \([13]\). Substituting \([13]\) into Eq. \([11]\) and using the condition \([16]\), we obtain the following first order coupled differential matrix equations

\[
\partial_r F_{[\ell][\ell']}^{(\pm)}(k, r) = \pm \frac{h_\ell^{(\pm)}(kr)}{2ik} \sum_{[\ell'']} W_{[\ell][\ell''][\ell']} (r) \left\{ h_{\ell''}^{(+)}(kr)F_{[\ell'][\ell'']}^{(+)}(k, r) + h_{\ell''}^{(-)}(kr)F_{[\ell'][\ell'']}^{(-)}(k, r) \right\}.
\]

As we show in the Appendix, the boundary condition \([14]\) can be rewritten as

\[
\lim_{r \to 0} \left[ \frac{j_\ell(kr)F_{[\ell][\ell']}^{(\pm)}(k, r)}{j_\ell(kr)} \right] = \delta_{[\ell][\ell']} ,
\]

and a series expansion for \( \|F_{[\ell][\ell']}^{(\pm)}(k, r)\| \) near the point \( r = 0 \) can be found iteratively as follows.
\[ F_{[\ell][\epsilon]}^{(\pm)(0)}(k, r) = \delta_{[\ell][\epsilon]}, \]
\[ F_{[\ell][\epsilon]}^{(\pm)(n+1)}(k, r) = \delta_{[\ell][\epsilon]} + \frac{1}{2ik} \int h_{[\ell]}^{(\pm)}(kr) \sum_{[\epsilon'] \epsilon} W_{[\ell][\epsilon']}(r) \]
\[ \times \left[ h_{[\ell]}^{(\ell')}(kr) F_{[\ell][\epsilon']}(n)(k, r) + h_{[\ell]}^{(-)}(kr) F_{[\ell][\epsilon']}(n)(k, r) \right] \, dr, \]

where the arbitrary constant for the indefinite integral is assumed to be zero. We shall give an explicit example for this expansion in Section IV.

In contrast to Eq. (14) the equations for the new unknown matrices \( \|F^{(\pm)}(k, r)\| \) are of first order. However the point \( r = 0 \) is generally a singular point because the Riccati–Hankel functions have the short range behaviour \( \sim r^{-\ell} \) and according to (3) the potential may also behave near this point as \( \sim r^{-(2-\varepsilon)} \), \( \varepsilon > 0 \). Therefore Eqs. (17) cannot be solved with the boundary conditions for \( \|F^{(\pm)}(k, r)\| \) at \( r = 0 \). Instead, we may use the analytical solutions of them in a small interval \( (0, \delta] \) (in the form of the above series expansions) and impose the boundary conditions at \( r = \delta \).

Certain elements of the matrices \( \|F^{(\pm)}(k, r)\| \) could diverge when \( r \to 0 \) (see the Appendix). This, however, does not cause any problem in the iterative procedure (20) since the integration is represented by an indefinite integral. It is emphasised that although certain elements of \( \|F^{(\pm)}\| \) diverge, the matrix \( \|\Phi\| \) always remains regular because at small \( r \) the matrices \( \|F^{(\pm)}\| \) converge to each other, that is they are transformed into some matrix \( \|A\| \) which is the same for both of them, \( \|F^{(\pm)}\| \to \|A\| \) (see the Appendix), and the singularities, if any, are compensated by the behaviour of the Riccati–Bessel function \( j_{\ell}(kr) \).

\[ \Phi_{[\ell][\epsilon']}(k, r) \to 0 \quad \text{as} \quad r \to 0 \quad \frac{1}{2} \left[ h_{[\ell]}^{(+)}(kr) + h_{[\ell]}^{(-)}(kr) \right] A_{[\ell][\epsilon']}(k, r) = j_{\ell}(kr) A_{[\ell][\epsilon']}(k, r). \]

The system of equations (17) together with the boundary values \( F_{[\ell][\epsilon']}(k, \delta) \approx F_{[\ell][\epsilon']}(N)(k, \delta) \) represent a well–defined differential problem, a solution of which gives the regular basis in the form (13).

**D. Jost matrices**

It can be proved (see the Appendix) that for \( \text{Im} \, k = 0 \) the right hand side of Eq. (14) vanishes when \( r \to \infty \). Since the corresponding derivatives also vanish, the functions \( F_{[\ell][\epsilon']}(k, r) \) become \( r \)–independent and thus, for momenta corresponding to the scattering states, we have

\[ \Phi_{[\ell][\epsilon']}(k, r) \to 0 \quad \text{as} \quad r \to \infty \quad \frac{1}{2} \left[ h_{[\ell]}^{(+)}(kr) F_{[\ell][\epsilon']}(k) + h_{[\ell]}^{(-)}(kr) F_{[\ell][\epsilon']}(k) \right] \]

where

\[ F_{[\ell][\epsilon']}(k) = \lim_{r \to \infty} F_{[\ell][\epsilon']}(k, r). \]
We may call these $r$–independent matrices $\|F^{(\pm)}\|$ as Jost matrices and the products $h^{(\pm)}(kr)F^{(\pm)}(k,r)$, which behave asymptotically like $\sim e^{\pm ikr}$, as Jost solutions.

For complex values of $k$ the above limits generally exist in different domains of the complex $k$–plane, namely, $F^{(+)}_{[\ell][\ell']}(k)$ in the lower half (Im $k \leq 0$) while $F^{(-)}_{[\ell][\ell']}(k)$ in the upper half (Im $k \geq 0$). This is because, according to Eq. (17), the derivatives $\partial_r F^{(\pm)}(k,r)$ are proportional to $h^{(\pm)}(kr)$ with

\[
h^{(\pm)}(kr) \xrightarrow{r \to \infty} \mp i \exp \left[ \pm i(kr - \ell \pi/2) \right]
\]  

vanishing in different domains of the $k$–plane, namely,

\[
h^{(+)}(kr) \xrightarrow{r \to \infty} 0, \quad \text{Im} (kr) > 0 , \tag{25}
\]
\[
h^{(-)}(kr) \xrightarrow{r \to \infty} 0, \quad \text{Im} (kr) < 0 . \tag{26}
\]

Thus, in general, the only area where the limits (23) simultaneously exist is the real axis \footnote{1 It can also be proved that both these limits exist at all spectral points corresponding to bound and resonance states (see the Appendix).}. However, for a particular class of short–range potentials (decaying exponentially or faster) the upper bound for the existence of $F^{(+)}$ is shifted upwards and the lower bound for $F^{(-)}$ downwards, which widens their common area to a band.

The difficulty concerning the existence of the limits (23), can be circumvented in the same way as for central potentials \footnote{1 It can also be proved that both these limits exist at all spectral points corresponding to bound and resonance states (see the Appendix)}. Indeed, the conditions (25) and (26) involve the imaginary part of the product $kr$ and not of the momentum alone. Therefore, if, for example, Im $(kr)$ is negative we can make it positive by using the complex rotation method which we describe next.

\section*{E. Complex rotation}

In this method the radius $r$ is replaced by a complex one, viz.,

\[ r = x \exp(i\theta) , \quad x \geq 0 , \quad 0 \leq |\theta| < \frac{\pi}{2} . \tag{27}\]

The idea of complex rotation of the coordinate is not new. Many years ago, during World War II, Hartree and his co-workers at Manchester university used such rotation to solve certain differential equations describing radio wave propagation in the atmosphere (for more details see Ref. \footnote{1 It can also be proved that both these limits exist at all spectral points corresponding to bound and resonance states (see the Appendix).}). Nowadays the complex rotation is widely used for locating quantum resonances by variational methods \footnote{1 It can also be proved that both these limits exist at all spectral points corresponding to bound and resonance states (see the Appendix).}. In contrast, our equations together with the complex rotation can be used to locate resonances in an exact way.

Applying the complex transformation (27) to Eq. (17), we obtain

\[ \text{---} \]
defined by the negative angle $\theta$ we may introduce a new pair of matrices $\mathbb{M}$. Thus we have $\text{Im} \ k \rho > 0$ negative, in calculating $\mathcal{F}^{(-)}$ with positive $\theta$ obeys the conditions (5, 6) along the ray (27), then the limit exists and is finite for all $k$ on and above the dividing line shown on Fig. 4. This line defined by the negative angle $\theta$ in the $k$–plane results from the rotation (27) in the $r$–plane with positive $\theta$.

If the potential matrix $\parallel W(r) \parallel$ is an analytic function of the complex variable $r$ and obeys the conditions (4, 5) along the ray (27), then the limit

$$\lim_{x \to \infty} F_{(\ell)[\ell]}^{(-)}(k, x e^{i\theta}) = \mathcal{F}_{(\ell)[\ell]}^{(-)}(k)$$

exists and is finite for all $k$ on and above the dividing line $[-\infty e^{-i\theta}, +\infty e^{-i\theta}]$ (for the relevant proof of this statement see the Appendix). At the same time the limit

$$\lim_{x \to \infty} F_{(\ell)[\ell]}^{(+)}(k, x e^{i\theta}) = \mathcal{F}_{(\ell)[\ell]}^{(+)}(k)$$

exists and is finite for all $k$ on and below the dividing line. Moreover, when the limits (29) and (30) exist the values of $\mathcal{F}_{(\ell)[\ell]}^{(\pm)}(k)$ are independent of the rotation angle $\theta$ as the Jost function is $r$–independent and hence $\theta$–independent. Thus, the limits (29) and (30) give a unique analytic continuation of the Jost matrices to the lower and upper halves of the complex $k$–plane respectively. To calculate the $\mathcal{F}_{(\ell)[\ell]}^{(\mp)}(k)$ for $\text{Im} \ k < 0$ we need to solve Eqs. (28) at a sufficiently large positive $\theta$, and the $\mathcal{F}_{(\ell)[\ell]}^{(\mp)}(k)$ for $\text{Im} \ k > 0$ at a sufficiently large negative $\theta$.

We note that though the ansatz (13) is suitable for large distances (see forth the next section), it is not good for numerical calculations in the vicinity of $r = 0$. Indeed, near this point the singularities of $h_{k}^{(+)}(kr)$ and $h_{k}^{(-)}(kr)$ are cancelled. Although this does not cause formally any problem, in numerical calculations the cancellation of singularities is always a source of possible numerical errors. These errors increase with increasing $\ell$ since in this case $h_{k}^{(\pm)}(kr)$ becomes more singular. Therefore, for larger $\ell$ the point $r = \delta$ must be shifted further from the origin. This in turn, requires more iterations of Eq. (20) to obtain the boundary values $F_{\ell e^{i\theta}(k, \delta)}$ to a required accuracy.

Eq. (21) hints to another way to handle numerically the boundary condition problem. Since

$$\frac{1}{2}(h_{k}^{+} + h_{k}^{-}) = j_{\ell} \quad \text{and} \quad \frac{1}{2i}(h_{k}^{+} - h_{k}^{-}) = n_{\ell},$$

we may introduce a new pair of matrices

$$A_{(\ell)[\ell]}(k, r) \equiv \frac{1}{2} \left[ F_{(\ell)[\ell]}^{(+))(k, r)} + F_{(\ell)[\ell]}^{(-)}(k, r) \right],$$

$$B_{(\ell)[\ell]}(k, r) \equiv \frac{1}{2i} \left[ F_{(\ell)[\ell]}^{(+)}(k, r) - F_{(\ell)[\ell]}^{(-)}(k, r) \right],$$

(31)
which transform the ansatz (13) into the form
\[
\Phi_{\ell}[\epsilon](k, r) = j_\ell(kr)A_{\ell}[\epsilon](k, r) - n_\ell(kr)B_{\ell}[\epsilon](k, r),
\]
and the corresponding linear combination of equations (17) gives the alternative form
\[
\begin{align*}
\partial_r A_{\ell}[\epsilon](k, r) &= -\frac{n_\ell(kr)}{k} \sum_{\epsilon'} W_{\ell}[\epsilon'][\epsilon'](r) \left[ j_\ell(kr)A_{\ell'}[\epsilon'](k, r) - n_\ell'(kr)B_{\ell'}[\epsilon'](k, r) \right], \\
\partial_r B_{\ell}[\epsilon](k, r) &= -\frac{j_\ell(kr)}{k} \sum_{\epsilon'} W_{\ell}[\epsilon'][\epsilon'](r) \left[ j_\ell(kr)A_{\ell'}[\epsilon'](k, r) - n_\ell'(kr)B_{\ell'}[\epsilon'](k, r) \right].
\end{align*}
\]
Likewise, the iterative procedure (19, 20) transforms into
\[
A_{\ell}[\epsilon](k, r) = \delta_{\ell}[\epsilon], \quad B_{\ell}[\epsilon](k, r) = 0,
\]
\[
\begin{align*}
A_{\ell}[\epsilon](k, r) &= \delta_{\ell}[\epsilon] - \frac{1}{k} \int n_\ell(kr) \sum_{\epsilon'} W_{\ell}[\epsilon'][\epsilon'](r) \left[ j_\ell(kr)A_{\ell'}[\epsilon'](k, r) - n_\ell'(kr)B_{\ell'}[\epsilon'](k, r) \right] dr, \\
B_{\ell}[\epsilon](k, r) &= -\frac{1}{k} \int j_\ell(kr) \sum_{\epsilon'} W_{\ell}[\epsilon'][\epsilon'](r) \left[ j_\ell(kr)A_{\ell'}[\epsilon'](k, r) - n_\ell'(kr)B_{\ell'}[\epsilon'](k, r) \right] dr.
\end{align*}
\]
The representation of \(\|\Phi\|\) in terms of \(\|A\|\), \(\|B\|\) and \(\|F(\pm)\|\) is equivalent. From a practical point of view, however, it is more convenient to start the integration of Eqs. (33) from the boundary values \(A_{\ell}[\epsilon](k, \delta)\), \(B_{\ell}[\epsilon](k, \delta)\) and at some intermediate point \(r_{int}\) (far enough from the origin) to go over to Eqs. (17) with starting values \(F_{\ell}(\pm)(k, r_{int})\) obtained from \(A_{\ell}[\epsilon](k, r_{int})\) and \(B_{\ell}[\epsilon](k, r_{int})\) via the linear combinations (31).

One may argue that we can abandon equations (17) altogether and integrate instead Eq. (33) on the whole interval \([\delta, r_{max}]\). However, \(\|F(\pm)(k, r)\|\) and \(\|F(\pm)(k, r)\|\) have finite limits \((r \to \infty)\) in different domains of the complex \(k\)-plane (below and above the dividing line respectively). The only points where they have limits simultaneously are the spectral points and the dividing line itself. And since \(\|A\|\) and \(\|B\|\) involve both \(\|F(\pm)\|\), they have limits only at these points. Therefore, to obtain the Jost matrix we should start at small \(r\) with Eq. (33) and finish at large \(r_{max}\) with Eq. (17).

### III. PHYSICAL SOLUTIONS

In what follows we shall describe how we can obtain a physical solution from the regular basis. In general, each column representing a physical solution is a linear combination of the basic columns,
\begin{align*}
u_{\ell}(k, r) &= \sum_{[\ell']} \Phi_{\ell}[\ell'](k, r)c_{[\ell']}, \quad (36) \\
u_{\ell'[\ell]}(k, r) &= \sum_{[\ell'\ell']} \Phi_{\ell'[\ell\ell']}(k, r)c_{[\ell'\ell']} \end{align*}

with the coefficients $\|c\|$ defined by the physical boundary condition (10) at large distances.

**A. Bound states**

The bound state wave function vanishes at large distances as

\[ \sum_{[\ell']} \Phi_{\ell}[\ell'](k, r)c_{[\ell']} \rightarrow_{r \to \infty} N_{[\ell]} e^{-|k|r} \rightarrow_{r \to \infty} 0, \]

where $N_{[\ell]}$ are the asymptotic normalisation constants. In this equation the function $\Phi_{\ell}[\ell'](k, r)$ can be replaced by its asymptotic form (22), i.e.,

\[ \frac{1}{2} \sum_{[\ell']} \left[ h_\ell^{(+)}(kr)F_{[\ell][\ell']}(k) + h_\ell^{(-)}(kr)F_{[\ell][\ell']}(k) \right] c_{[\ell']} \rightarrow_{r \to \infty} 0. \quad (37) \]

For bound states $\text{Im} \ k > 0$ and the Riccati–Hankel function $h_\ell^{(+)}(kr)$ decays exponentially while $h_\ell^{(-)}(kr)$ grows exponentially. Therefore the condition (37) can be fulfilled only if we find coefficients $c_{[\ell]}$ such that the diverging functions $h_\ell^{(-)}(kr)$ of different columns cancel out, that is, if

\[ \sum_{[\ell']} F_{[\ell][\ell']}(k)c_{[\ell']} = 0. \quad (38) \]

This system of homogeneous linear equations has a nontrivial solution if and only if

\[ \det \|F(\ell')\| = 0. \quad (39) \]

Therefore, we can locate all possible bound states by looking for zeros $k_0$ of the Jost–matrix determinant on the positive imaginary axis (see Fig. 1). For each zero $k_0$ thus found, the coefficients $c_{[\ell]}$ are then uniquely determined by the system (38) apart from a general normalisation factor which is finally fixed when the physical wave function,

\[ \Psi_{k_0JM}(\vec{r}) = \frac{1}{2} \sum_{[\ell][\ell']} \mathcal{J}_{[\ell][\ell']}(\vec{r}) \left[ h_\ell^{(+)}(k_0r)F_{[\ell][\ell']}(k_0, r) + h_\ell^{(-)}(k_0r)F_{[\ell][\ell']}(k_0, r) \right] c_{[\ell']}, \quad (40) \]

is normalised. The contribution of each element of the column

\[ u_{[\ell]}(k_0, r) = \frac{1}{2} \sum_{[\ell']} \left[ h_\ell^{(+)}(k_0r)F_{[\ell][\ell']}(k_0, r) + h_\ell^{(-)}(k_0r)F_{[\ell][\ell']}(k_0, r) \right] c_{[\ell']} \quad (41) \]

into the normalisation integral represents what is usually called the percentage of the corresponding partial wave.
B. Scattering states

The scattering states normalised to the $\delta$–function,
\[ \langle \Psi_{k\mu} | \Psi_{k's'\mu'} \rangle = \delta(k - k') \delta_{ss'} \delta_{\mu\mu'}, \]
are defined by the following asymptotic condition
\[ \Psi_{k\mu}(\vec{r}) \xrightarrow{r \to \infty} \frac{1}{(2\pi)^{3/2}} \left[ e^{ik\vec{r} \cdot \hat{r}} \chi_{s\mu} + \frac{e^{i\pi}}{r} \sum_{s'\mu'} f_{s'\mu's\mu}(k, \vec{r}) \chi_{s'\mu'} \right], \tag{42} \]
where $f_{s'\mu's\mu}(\vec{k}', \vec{k})$ is the scattering amplitude. The partial wave decomposition of Eq. (42) gives for the boundary condition (10) (see Ref. [1])
\[ u_{J}[\ell][\ell'](k, r) \xrightarrow{r \to \infty} \frac{1}{2} \left[ h_{\ell'}^{|-\rangle}(kr) \delta_{\ell'\ell} + h_{\ell'}^{|+\rangle}(kr) S_{J}^{J'}[\ell][\ell'](k) \right]. \tag{43} \]

Therefore the choice of our ansatz (13) for the regular basis is natural and suitable not only for constructing the bound states but the scattering states as well. Indeed, comparing (43) with (22) we find that the coefficients $c_{J}[\ell][\ell']$ in (36) should be chosen as
\[ c_{J}[\ell][\ell'] = \| F_{J}^{\ell}[\ell']^{J'}(k) \|^{-1}, \]
which gives us the $S$–matrix in the form
\[ \| S(k) \| = \| F_{J}^{\ell}[\ell']^{J'}(k) \| \cdot \| F_{J}^{\ell}[\ell'][\ell]\|^{-1}. \tag{44} \]

Thus, the normalised scattering wave function can be constructed from the regular basis as follows
\[ \Psi_{k\mu}(\vec{r}) = \frac{1}{\sqrt{2\pi kr}} \sum_{JM} \sum_{[\ell']} \sum_{[\ell'']} Y_{JM}^{\ell[J}[\ell']^{J'}(\hat{r}) u_{J}[\ell'][\ell]\| \left\{ h_{\ell'}^{\ell'}(kr) F_{J}[\ell'][\ell']^{J'}(k, r) + h_{\ell'}^{\ell'}(kr) F_{J}[\ell'][\ell']^{J'}(k, r) \right\} \| F_{J}^{\ell}[\ell'][\ell]\|^{-1}. \tag{45} \]

The scattering phase shifts together with the mixing parameters can be found from the $S$–matrix given by Eq. (44).

C. Resonances

The resonance (or Siegert) states are described by wave functions which at large distances have only outgoing spherical waves
\[ \Psi_{kJ[M}(\vec{r}) = \frac{1}{\sqrt{2\pi kr}} \sum_{[\ell]} Y_{JM}^{\ell}[\ell]\| u_{J}[\ell](k, r) \xrightarrow{r \to \infty} e^{i\pi} \| \sim \frac{e^{i\pi}}{r}. \tag{46} \]

More precisely, the resonant boundary condition at large $r$ is
\[ u_{[\ell]}^J(k, r) \xrightarrow{r \to \infty} N_{[\ell]}^J(k) h_{\ell}^{(+)}(kr), \] (47)

where \( N_{[\ell]}^J(k) \) are the partial wave normalisation constants. Since there is not a generally accepted convention about the normalisation of Siegert states, the \( N_{[\ell]}^J(k) \) may involve an arbitrary coefficient. Solutions of the Schrödinger equation, with the long–range behaviour (47), may exist only at discrete points of the complex \( k \)–plane, situated below the real axis (see Fig. 1). The corresponding radial wave functions are regular at the origin and are therefore linear combinations of the regular basis

\[ u_{[\ell]}(k, r) = \frac{1}{2} \sum_{[\ell]} \left\{ h_{\ell}^{(+)}(kr) F_{[\ell][\ell']}^{(+)}(k, r) + h_{\ell}^{(-)}(kr) F_{[\ell][\ell']}^{(-)}(k, r) \right\} c_{[\ell']} \] (48)

This equation can be used to locate resonances. Similarly to the bound states, we simply require that

\[ \lim_{r \to \infty} \sum_{[\ell']} F_{[\ell][\ell']}^{(-)}(k, xe^{i\theta}) c_{[\ell']} = 0, \quad \theta > 0, \] (49)

which means that \( u_{[\ell]}(k, r) \) is expressed only in terms of \( h_{\ell}^{(+)}(kr) \) at large distances. Since \( \theta \) can be chosen such that \( \text{Im} \, kr > 0 \), the Riccati–Hankel function \( h_{\ell}^{(+)}(kr) \) decays exponentially when \( |r| \to \infty \). This in turn means that the Siegert states are quadratically integrable according to (47) and hence they acquire the same properties as the bound states. Therefore, with the coordinate rotation the bound and resonance states can be treated in the same way. In particular, the position of a resonance is defined by Eq. (39), and its (rotated) wave function by Eq. (40) where \( r \) is now complex.

IV. EXAMPLES

In order to demonstrate the effectiveness of the method we consider as an example the nucleon–nucleon (NN) interaction in the triplet spin–state, i.e., when the total spin \( s = 1 \). From the Pauli principle it follows that \( s \) is conserved (see for example Ref. [15]), and thus the sum over \( [\ell] \) is reduced to \( \sum \ell \). The triplet NN potential can couple only at most two partial waves, with \( \ell = J - 1 \) and \( \ell = J + 1 \), as the state with \( \ell = J \) has different parity and therefore must be excluded. We consider here the even state of two nucleons with \( J = 1 \), in which they can form the deuteron. The partial wave decomposition of this state consists of coupled \( S \) and \( D \) waves.
The corresponding NN potential includes the following three most important terms

\[ V(\vec{r}) = V_c(r) + V_t(r)S_{12} + V_{ls}(r)(\vec{\ell} \cdot \vec{s}), \]

known as the central, tensor, and spin–orbit potentials. The second term contains the tensor operator

\[ S_{12} = \frac{3}{r^2}(\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r}) - (\vec{\sigma}_1 \cdot \vec{\sigma}_2) \]

which is responsible for the coupling of different partial waves. This is clearly seen from the structure of the matrix \( \|W\| \) defined by Eq. (4), which in the case of \( s = 1, J = 1, \) and \( \pi = +1 \) reads (see for example Ref. [1])

\[
\begin{pmatrix}
W_{00} & W_{02} \\
W_{20} & W_{22}
\end{pmatrix}
\equiv
2m
\begin{pmatrix}
V_c & 2\sqrt{2}V_t \\
2\sqrt{2}V_t & V_c - 2V_t - 3V_{ls}
\end{pmatrix},
\]

(51)

where the subscripts of \( \|W_{\ell\ell'}\| \) correspond to the two partial waves \( \ell = 0 \) and \( \ell = 2. \)

In accordance with the restriction (5) we may use at short distances the series expansion

\[ W_{\ell\ell'}(r) \xrightarrow{r \to 0} a_{\ell\ell'}r^{-1} + b_{\ell\ell'} + c_{\ell\ell'}r + \ldots, \]

(52)

which is general enough to include potentials having a soft core \( (a_{\ell\ell'} \neq 0). \)

Using (52) we can obtain the corresponding expansions for \( A_{\ell\ell'}(k, r) \) and \( B_{\ell\ell'}(k, r) \) via the iterative procedure (34, 35) which are needed to impose the boundary conditions \( A_{\ell\ell'}(k, \delta) \) and \( B_{\ell\ell'}(k, \delta) \) at a small \( \delta. \) These expansions near the point \( r = 0 \) can be obtained in an explicit form. For this we replace the Riccati functions in the indefinite integrals (35) by their series expansions [12]

\[
j_0(kr) = kr - \frac{(kr)^3}{6} + \frac{(kr)^5}{120} - \cdots,
\]

\[
j_2(kr) = \frac{(kr)^3}{15} - \frac{(kr)^5}{210} + \frac{(kr)^7}{7560} - \cdots,
\]

\[
n_0(kr) = -1 + \frac{(kr)^2}{2} - \frac{(kr)^4}{24} + \cdots,
\]

\[
n_2(kr) = -\frac{3}{2} \frac{(kr)^2}{8} - \frac{1}{2} - \frac{(kr)^2}{8} - \cdots.
\]

Substituting (34) into (35) and performing the integrations over \( r \) for each element of the matrices \( \|A\| \) and \( \|B\| \) we obtain

\[
\|A^{(1)}(k, r)\| = \begin{pmatrix}
1 + a_{00}r & \frac{a_{02}k^2}{45}r^3 \\
-\frac{3a_{20}}{k^2}r^{-1} & 1 + \frac{a_{22}}{5}r
\end{pmatrix},
\]

\[
\|B^{(1)}(k, r)\| = \begin{pmatrix}
-\frac{a_{00}k^2}{2}r^2 & -\frac{a_{02}k^3}{60}r^4 \\
\frac{a_{20}k^3}{60}r^4 & -\frac{a_{22}k^5}{1350}r^6
\end{pmatrix},
\]

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where we retain only one additional term in each matrix element. For the second iteration we get

\[
\|A^{(2)}(k, r)\| = \begin{pmatrix} 1 + a_{00} r + \frac{\zeta_{00}}{2} r^2 & a_{02} k^2 \frac{r^3}{45} + \frac{k^2 \zeta_{02}}{60} r^4 \\ -3a_{20} k^2 r^{-1} + \frac{3\zeta_{20}}{k^2} \ln r & 1 + a_{22} r^2 + \frac{\zeta_{22}}{10} r^2 \end{pmatrix},
\]

\[
\|B^{(2)}(k, r)\| = \begin{pmatrix} \frac{a_{00} k}{2} - \frac{k \zeta_{00}}{3} r^3 & a_{02} k^3 \frac{r^4}{60} - \frac{k^3 \zeta_{02}}{75} r^5 \\ -a_{20} k^3 \frac{r^4}{60} + \frac{k^3 \zeta_{20}}{75} r^5 & a_{22} k^5 \frac{r^6}{1350} - \frac{k^5 \zeta_{22}}{1575} r^7 \end{pmatrix},
\]

where the constants \(\zeta_{\ell\ell'}\) are defined as

\[
\left( \begin{array}{cc} \zeta_{00} & \zeta_{02} \\ \zeta_{20} & \zeta_{22} \end{array} \right) = \left( \begin{array}{cc} \frac{a_{00}^2}{2} + b_{00} - \frac{a_{02} a_{20}}{4} & \frac{a_{00} a_{02}}{12} + b_{02} + \frac{a_{02} a_{22}}{6} \\ \frac{a_{20} a_{00}}{2} + b_{20} - \frac{a_{22} a_{20}}{4} & \frac{a_{20} a_{02}}{12} + b_{22} + \frac{a_{22}^2}{6} \end{array} \right).
\]

The iterations can be continued in the same manner with each iteration adding a new term to each matrix element having a higher power of \(r\) than the previous one. All matrix elements of \(\|A\|\) and \(\|B\|\) are regular when \(r \to 0\) except for the left bottom corner element of \(\|A\|\). It has two singular terms, \(\sim r^{-1}\) and \(\sim \ln r\). The next iteration however gives for it a vanishing term of the kind \(\sim r \ln r\), and all subsequent terms are vanishing even faster.

The above expansions illustrate the fact that at small \(r\) the matrices \(\|F^{(+)}\|\) and \(\|F^{(-)}\|\) converge to each other. Indeed, since \(\|B\|\) is infinitesimal as compared to \(\|A\|\) the second term in the linear combinations \(\|F^{(+)}\| = \|A\| \pm i\|B\|\) vanishes when \(r \to 0\).

The singularities of the matrix \(\|A_{[\ell][\ell']}\|\) reflects the main difficulty of the theory of coupled partial waves, which precluded its development in the past. As we show in the Appendix, the matrix elements of \(\|F^{(+)}\|\) with \(\ell > \ell'\) are always singular at \(r = 0\) if the potential is nonzero at that point. Despite this the functions \(\Phi_{[\ell][\ell']}(k, r)\) remain always regular because in Eq. (32) the singularity of \(A_{[\ell'][\ell']}(k, r)\) is compensated by \(j_{\ell}(kr)\). In our case we have

\[
\|\Phi\| = \begin{pmatrix} j_0 & 0 \\ 0 & j_2 \end{pmatrix} \begin{pmatrix} A_{00} & A_{02} \\ A_{20} & A_{22} \end{pmatrix} - \begin{pmatrix} n_0 & 0 \\ 0 & n_2 \end{pmatrix} \begin{pmatrix} B_{00} & B_{02} \\ B_{20} & B_{22} \end{pmatrix}
\]

and therefore the singular term \(A_{20}(k, r)\) appears only in the product \(j_2(kr)A_{20}(k, r)\) which vanishes at the origin as \(\sim r^2\). Substituting the series expansions of all functions involved into Eq. (53) we obtain
\[ \Phi(k; r) \xrightarrow{r \to 0} \left( \begin{array}{c} kr + \frac{a_0 k^2 r^2}{2} + \frac{\zeta_0 k^3}{6} r^3 + \mathcal{O}(r^4 \ln r) \\ -\frac{a_2 k^2 r^2}{4} + \frac{\zeta_2 k^3}{5} r^3 + \mathcal{O}(r^4 \ln r) \end{array} \right) \frac{a_0 k^3}{180} r^4 + \frac{\zeta_0 k^3}{300} r^5 + \mathcal{O}(r^6) \]

(54)

which explicitly demonstrates that our regular basis obeys the boundary condition (14) and, as mentioned in Sec. II, in each row the convergence to zero increases from left to right while in each column the diagonal elements have the lowest vanishing speed. The linear independence of these columns is also apparent. As far as the off-diagonal elements are concern, even the leading terms of them depend on the behaviour of the potential, i.e., it is impossible to specify the boundary condition for them in a general form independently from the potential.

Using a quite different approach, Palumbo in Ref. [10] derived recurrence formulae for direct constructing the series expansion of the regular basis for the potentials of the type (52). Having performed few iterations of the Palumbo’s formulae, we found that they generate the same terms which are given in Eq. (54). This is yet another confirmation that our iterative procedures (19, 20) and (34, 35) are correct.

In order to test the proposed method numerically, we chose two different NN–potentials of the type (52). The first one is the Reid soft core potential (RSC) [16], which for \( J = 1, s = 1, \pi = +1 \) has the following form

\[
V_c(r) = h_0 e^{-\alpha r} + h_1 e^{-2\alpha r} + h_2 e^{-4\alpha r} + h_3 e^{-6\alpha r},
\]

\[
V_t(r) = h_0 \left\{ \left( 1 + \frac{3}{\alpha r} + \frac{3}{\alpha r^2} \right) e^{-\alpha r} - \left[ \frac{12}{\alpha r^2} + \frac{3}{\alpha r^3} \right] e^{-4\alpha r} \right\} +
\]

\[
+ h_4 e^{-4\alpha r} + h_5 e^{-6\alpha r},
\]

\[
V_{ls}(r) = h_6 e^{-4\alpha r} + h_7 e^{-6\alpha r},
\]

with

\[
\begin{align*}
&h_0 = -10.463 \text{ MeV}, \quad h_1 = 105.468 \text{ MeV}, \quad h_2 = -3187.8 \text{ MeV}, \\
&h_3 = 9924.3 \text{ MeV}, \quad h_4 = 351.77 \text{ MeV}, \quad h_5 = -1673.5 \text{ MeV}, \\
&h_6 = 708.91 \text{ MeV}, \quad h_7 = -2713.1 \text{ MeV}, \quad \alpha = 0.7 \text{ fm}^{-1}.
\end{align*}
\]

The second potential used, is the Moscow potential [17],

\[
\begin{align*}
V_c(r) &= V_1 e^{-\gamma r^2} + V_2 \left( 1 - e^{-\gamma r} \right) \frac{e^{-\beta r}}{\beta r}, \\
V_t(r) &= V_2 \left[ 1 + \frac{3}{\beta r} + \frac{3}{(\beta r)^2} \right] \left( 1 - e^{-\gamma r} \right)^3 \frac{e^{-\beta r}}{\beta r}, \\
V_{ls}(r) &\equiv 0,
\end{align*}
\]

(56)
with
\[ V_1 = -466.74 \text{ MeV}, \quad V_2 = -10.69 \text{ MeV}, \]
\[ \beta = 0.6995 \text{ fm}^{-1}, \quad \gamma = 3 \text{ fm}^{-1}, \quad \eta = 1.6 \text{ fm}^{-2}. \]

The RSC potential has a strong repulsion at small distances,
\[
\|a_{\ell\ell'}\| = \frac{2m}{\alpha} \left( \begin{array}{c}
    h_0 + h_1 + h_2 + h_3 \\
    2\sqrt{2}(h_4 + h_5 + 23.5h_0) \\
    2\sqrt{2}(h_4 + h_5 + 23.5h_0)
\end{array} \right)
\]
\[
\approx \frac{2m}{\alpha} \left( \begin{array}{cc}
    6832 \text{ MeV} & -4434 \text{ MeV} \\
    -4434 \text{ MeV} & 15979 \text{ MeV}
\end{array} \right).
\]

In contrast the Moscow potential has very strong attraction instead and sustains, apart from the deuteron bound state, a very deep bound state known as Pauli Forbidden State (PFS). In this case the expansion (52) begins from the second term,
\[
\|b_{\ell\ell'}\| = 2m \left( \begin{array}{c}
    V_1 + V_2 \frac{\gamma}{\beta} \\
    6\sqrt{2}V_2 \frac{\gamma^3}{\beta^3} \\
    6\sqrt{2}V_2 \frac{\gamma^3}{\beta^3}
\end{array} \right)
\]
\[
\approx 2m \left( \begin{array}{cc}
    -513 \text{ MeV} & -7156 \text{ MeV} \\
    -7156 \text{ MeV} & 4547 \text{ MeV}
\end{array} \right).
\]

Both potentials describe the deuteron properties and the \(np\)–scattering quite well despite their completely different short range behaviour.

To begin with we consider real energies corresponding to bound and scattering states. We integrated Eqs. (17) by the Runge–Kutta method from \(r_{\text{min}} = 10^{-4} \text{ fm}\) to \(r_{\text{int}} = 1 \text{ fm}\) with the boundary conditions \(\|A^{(4)}(k, r_{\text{min}})\|\) and \(\|B^{(4)}(k, r_{\text{min}})\|\). Then from \(r_{\text{int}} = 1 \text{ fm}\) we integrated Eqs. (17) up to \(r_{\text{max}} = 20 \text{ fm}\) where the functions \(F^{(\pm)}(k, r)\) attain their limits (23). Repeating such calculations with different values of the momentum \(k\) corresponding to points on the positive imaginary axis, we found that the equation
\[
\det \|F^{(-)}(k, r_{\text{max}})\| = 0 \tag{57}
\]
is fulfilled at the points \(k_0\) given in Table I. The binding energies and the percentages of the \(D\)–waves (\(D\%\)) are also given in this table. For comparison Table I contains the energies and \(D\%\) obtained originally in Refs. [14–18] by the authors that constructed these potentials. The other observables such as the mean square radius and the electric quadrupole moment of the deuteron are also the same as given in Refs. [16–17]. Due to the presence of the deep unphysical PFS state in the Moscow potential the deuteron state is an excited one and therefore its wave function has a node at \(r_c \sim 0.59 \text{ fm}\).

For real positive \(k\), i.e., for scattering states, we performed calculations with the same \(r_{\text{min}}, r_{\text{int}},\) and \(r_{\text{max}}\). According to Eq. (44) the product
\[\|F^{(+)}(k, r_{\text{max}})\| \cdot \|F^{(-)}(k, r_{\text{max}})\|^{-1} = \|S(k)\|\]
gives us the \(S\)–matrix which contains information about the scattering observables. The nucleon–nucleon \(S\)–matrix usually is parametrised in terms of the so–called \(\text{bar}\) phase shifts and mixing parameter, introduced in Ref. [14], as follows
\[
\begin{pmatrix}
    S_{00} & S_{02} \\
    S_{20} & S_{22}
\end{pmatrix} = \begin{pmatrix}
    e^{i\delta_0} \cos 2\xi & ie^{i(\delta_0 + \delta_2)} \sin 2\xi \\
    ie^{i(\delta_0 + \delta_2)} \sin 2\xi & e^{2i\delta_2} \cos 2\xi
\end{pmatrix}.
\]
From this matrix equation one gets

\[ \delta_0 = \frac{\ln S_{00}}{2i} \sqrt{1 - \frac{S_{02}^2}{S_{00}S_{22}}}, \]

\[ \delta_2 = \frac{\ln S_{22}}{2i} \sqrt{1 - \frac{S_{02}^2}{S_{00}S_{22}}}, \]

\[ \bar{\varepsilon} = \frac{1}{4} \arccos \left( \frac{S_{00}S_{22} + S_{02}^2}{S_{00}S_{22} - S_{02}^2} \right). \]

The obtained phase shifts and mixing parameters are in agreement with the values given in Ref. [16], for all collision energies examined (up to \( E_{c.m.} = 176 \) MeV). For example, at \( E_{c.m.} = 12 \) MeV \( (k = 0.53793 \text{ fm}^{-1}) \) the RSC potential gives

\[ \left\| F^{(\pm)}(k, r_{\text{max}}) \right\| = \begin{pmatrix} 0.16247 \times 10^{11} \mp i0.18386 \times 10^{12} & -0.60905 \times 10^5 \pm i0.68923 \times 10^6 \\ -0.13390 \times 10^{13} \pm i0.61083 \times 10^{11} & 0.50194 \times 10^7 \mp i0.22898 \times 10^6 \end{pmatrix} \]

and

\[ \left\| S(k) \right\| = \begin{pmatrix} -0.95640 + i0.28507 & -0.06232 + i0.01229 \\ -0.06232 + i0.01229 & 0.99303 - i0.09933 \end{pmatrix}. \]

From the latter \( S \)-matrix we obtain the following scattering parameters

\[ \bar{\delta}_0 = 1.4288, \quad \bar{\delta}_2 = -0.04995, \quad 2\bar{\varepsilon} = 0.06357, \]

which practically the same with those obtained by Reid [16]

\[ \bar{\delta}_0 = 1.426, \quad \bar{\delta}_2 = -0.050, \quad 2\bar{\varepsilon} = 0.064, \]

via direct a solution of the Schrödinger equation.

The Moscow potential at the same energy gives different Jost matrices,

\[ \left\| F^{(\pm)}(k, r_{\text{max}}) \right\| = \begin{pmatrix} -361.16 \pm i4347.4 & -0.08458 \pm i1.0183 \\ 30864 \mp i1423.1 & 7.2291 \mp i0.33331 \end{pmatrix}, \]

but practically the same \( S \)-matrix

\[ \left\| S(k) \right\| = \begin{pmatrix} -0.95557 + i0.28772 & -0.06283 + i0.01252 \\ -0.06283 + i0.01252 & 0.99268 - i0.10059 \end{pmatrix}. \]

and therefore the same phase shifts and mixing parameter

\[ \bar{\delta}_0 = 1.4275, \quad \bar{\delta}_2 = -0.05059, \quad 2\bar{\varepsilon} = 0.06411. \]

\[ ^2 \text{The calculated } \left\| F^{(+)}(k, r_{\text{max}}) \right\| \text{ and } \left\| F^{(-)}(k, r_{\text{max}}) \right\| \text{ are complex conjugate to each other at least within five digits} \]
The huge values of the above Jost matrix elements are due to the behaviour of the potentials at small distances, which generates large values of the derivatives \( \partial_r \| F^{(\pm)}(k, r) \| \) that pushes up the absolute values of the functions \( F^{(\pm)}(k, r) \). To demonstrate an opposite example, we solved Eqs. (17) at the same energy \((E_{c.m.} = 12 \text{ MeV})\) with a rudimentary nucleon–nucleon potential (also in the deuteron channel) consisting of two Yukawa–type terms \([20]\),

\[
V(r) = v_c \frac{\exp(-\omega r/\rho_c)}{r/\rho_c} + v_t \frac{\exp(-\omega r/\rho_t)}{r/\rho_t} S_{12},
\]

\[
v_c = -22.7 \text{ MeV}, \quad v_t = -10.9 \text{ MeV}, \quad \omega = 2.12, \quad \rho_c = 2.47 \text{ fm}, \quad \rho_t = 3.68 \text{ fm}.
\]

Like the RSC it is singular at \( r = 0 \), but the coefficients \( \| a_{\ell \ell'} \| = 2m\rho_c \begin{pmatrix} -22.7 \text{ MeV} & -45.9 \text{ MeV} \\ -45.9 \text{ MeV} & 9.8 \text{ MeV} \end{pmatrix} \) for its expansion \((52)\) are in two orders of magnitude less than those for the RSC potential. As a result the Jost matrices calculated at \( E_{c.m.} = 12 \text{ MeV} \) are

\[
\| F^{(\pm)}(k, r_{\max}) \| = \begin{pmatrix} 0.27328 \pm i0.87845 & 0.11204 \pm i0.23730 \\ 3.8437 \mp i0.37653 & 1.6876 \mp i0.15658 \end{pmatrix},
\]

while the \( S \)-matrix is

\[
\| S(k) \| = \begin{pmatrix} -0.98755 + i0.10546 & 0.11564 - i0.015980 \\ 0.11564 - i0.015980 & 0.97914 - i0.16631 \end{pmatrix}
\]

are \( \tilde{\delta}_0 = 1.53, \tilde{\delta}_2 = -0.0847, \) and \( \tilde{\epsilon}_0 = 0.117 \).

So far we dealt with momenta on and above the real axis \((\text{Im } k \geq 0)\) and therefore the coordinate rotation \((27)\) was not needed. Consider now a point \( k \) which is under the real axis. To obtain the Jost matrix \( \| F^{(-)}(k) \| \) in this domain of the \( k \)-plane, we must integrate the rotated equations \((28)\) (with \( \theta > 0 \)) along the real variable \( x = |r| \). Similarly to the case with \( \theta = 0 \), in the immediate vicinity of the point \( x = 0 \) it is convenient, for numerical reasons, to replace \( \| F^{(\pm)} \| \) by their linear combinations \((31)\) and the equations \((28)\) by the corresponding linear combinations of them. The resulting rotated equations for \( \| A \| \) and \( \| B \| \) as well as the rotated iterative equations follow immediately from \((33), (34), \) and \((35)\) after simple replacement of \( r \) by \( x \exp(i\theta) \).

To demonstrate the ability of the method to deal with momenta of the fourth quadrant of the \( k \)-plane, we calculated the Jost matrix for the RSC potential at \( k = 0.5 \exp(-i0.3\pi) \text{ fm}^{-1} \), i.e., at \( E_{c.m.} \approx (-3.20 - i9.86) \text{ MeV} \), with three different values of the rotation angle: \( \theta = 0, 0.35\pi, 0.4\pi \). The results obtained are given in Table II. The first line of this table demonstrates that the unrotated equations cannot give a correct \( \theta \)-independent Jost matrix when \( \text{Im } k < 0 \). The matrix obtained with \( \theta = 0 \) is also \( r \)-dependent, i.e., has no limit when \( |r| \to \infty \). If however \( \theta \) is large enough, such that \( \text{Im } kr \geq 0 \) and the point \( k \) is
above the dividing line, then \( \| F^-(k, x_{\text{max}} e^{i\theta}) \| \) does not depend on \( \theta \) (compare the second and third lines of the table) and \( x_{\text{max}} \). To achieve the \( x_{\text{max}} \)-independence when \( \theta \neq 0 \), we have to go further afield because the potential vanishes along the \( x \exp(i\theta) \) slower than along the real \( r \). Thus, the results given in Table II were obtained with \( x_{\text{max}} = 50 \text{ fm} \).

The number of digits which are unchanged under the rotation show the accuracy achieved. In this connection it is interesting to note that the accuracy of the second column of the Jost matrix as well as of the determinant turn out to be always much higher than that of the Jost matrix first column. This is exemplified by the two last lines of Table II. It is interesting to know that the correct value of the determinant can be obtained even with crude boundary conditions and large tolerance of the Runge–Kutta procedure. Thus, the correct binding energy of the deuteron (given in Table I) can be obtained even with boundary conditions \( \| A^{(1)}(k, r_{\text{min}}) \| \) and \( \| B^{(1)}(k, r_{\text{min}}) \| \) when the first column of \( \| F^-(k, r_{\text{max}}) \| \) is even wrong. The only explanation for this is that somehow both elements of this column get the same erroneous term which cancel out in the determinant. This observation means that the procedure of locating spectral points is less demanding and less delicate than the calculations of the corresponding wave functions.

None of the potentials (55, 56, 58) generates resonances (at least at reasonably low energies). To the best of our knowledge, non-central potentials generating resonances have not been published yet. Thus, in order to demonstrate the ability of our method to locate Siegert states we constructed an artificial potential with a rich spectrum. For this we used the well–known central potential

\[ V_c(r) = 7.5r^2 \exp(-r) , \]

which is widely used as a testing case for new methods that locate resonances (see for example Refs. [7, 21–23]). It is usually assumed that this potential is given in atomic units. In order to be consistent, however, with the potentials used in this work, we assume that it is given here in MeV. Then for \( \hbar^2/2m = 1/2 \text{ MeV fm}^2 \), the numerical values of the resonance energies are the same in MeV and in atomic units.

This potential generates a sequence of \( S \)-wave resonances (see Ref. [7]) which cannot be significantly displaced if we add very weak interaction in the \( D \)-wave and a weak \( S-D \) coupling. Thus the non–central potential coupling of the \( S \) and \( D \) partial waves which is represented by the matrix

\[ \| W_{\ell\ell'}(r) \| = 2m \begin{pmatrix} 7.5r^2 \exp(-r) & -\lambda r^2 \exp(-r) \\ -\lambda r^2 \exp(-r) & -\lambda r^2 \exp(-r) \end{pmatrix} , \]

should generate resonances at least when \( \lambda \) is small. Bound states can also be generated by increasing \( \lambda \) since we have chosen a negative sign for the \( D \)-wave potential and for the off–diagonal elements of the matrix (60).

Of course the use, as a testing case, of a potential with a weak \( D \)-wave and weak coupling is rather undesirable. Therefore, we gradually increased \( \lambda \) up to the value \( \lambda = 15 \text{ MeV} \). The resulting spectrum is given in Table III and depicted in Fig. 2. It consists of eight bound
states and a sequence of resonances (we show only six of them, nearest to the real axis). By the large open circles in Fig. 2 we also show the positions of the first three resonances when \( \lambda = 0 \) which coincide with the resonances of the potential (59) found in Ref. [7]. The small open circles show their movement when \( \lambda \) is gradually increased in steps of \( \Delta \lambda = 1 \text{ MeV} \). The digits displayed in Table III are those which do not change when the rotation angle changes and thus they represent the accuracy of our calculations.

**V. CONCLUSIONS**

The present work is a continuation of a series of papers [4,6,7] in which a practical method for quantum mechanical calculations is developed. The method is based on direct calculations of the Jost function and Jost solutions and is a combination of the variable–constant method with the complex coordinate rotation. Here we have extended it to include non-central potentials.

The proposed method offers a unified way of treating bound, scattering, and resonance state problems. It is a powerful method which enables us to investigate the analytical properties of the Jost function in the complex momentum plane. This opens up new possibilities in locating resonances. Within this method the Siegert wave functions can be properly normalised. Even sub-threshold resonances can be located which is a difficult task for many other methods. Moreover the formalism presented can be easily extended to complex values of the angular momentum \( \ell \) and therefore Regge trajectories can also be located [7].

The wave function can be obtained in a form which guarantees its correct asymptotic behaviour for all three types of physical problems. In all cases the same accuracy can be achieved which can be reliably controlled by simply changing the rotation angle.

Despite the restriction (6), the potentials with Coulomb tails can be incorporated into the proposed method in a straightforward way as it was done in our previous publications [4,5]. To do this we need only to replace in all formulae the Riccati–Bessel functions by the corresponding Coulomb functions.

The method can be extended further: Firstly, to treat the \( N \)–body coupled hyperradial equations which differ from the two–body radial equations only by the possibility of having half–integer values of \( \ell \); secondly, to investigate the behaviour of the coupled partial waves when the angular momenta is complex valued; thirdly, to treat non-analytical and singular potentials, and fourthly to treat coupled channel problems with different thresholds. The work on all these extensions is under way.

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APPENDIX A: REGULAR BASIS

By definition, \( \|\Phi(k, r)\| \) is a regular basis (fundamental matrix) if it has the following three properties [1]:

i) Each column of \( \|\Phi_{[\ell'][\ell]}\| \) is a solution of Eq. (11),

ii) \( \Phi_{[\ell'][\ell]}(k, 0) = 0, \quad \forall \ [\ell'], [\ell], \)

iii) all columns of \( \|\Phi_{[\ell'][\ell]}\| \) are linearly independent.

Moreover, \( \|\Phi\| \) must be a square matrix since Eq. (11) has as many independent regular column–solutions as the column dimension [24].

1. Behaviour at short distances

The property ii) implies that the boundary condition (12) should be imposed at the point \( r = 0 \). Eq. (11), however, is singular at the origin, and consequently the existence and uniqueness theorem [24] is not valid at this point. This theorem is valid for all \( r \geq \delta > 0 \) for any arbitrary small \( \delta \). Hence, the matrix \( \|\Phi\| \) can be uniquely defined by \( \|\Phi(k, \delta)\| \) and \( \partial_r\|\Phi(k, \delta)\| \), while within the interval \([0, \delta]\), \( \|\Phi(k, r)\| \) (having the above three properties) can be obtained explicitly as follows. After multiplying by \( r^2 \) and using (5), Eqs. (11) decouple giving

\[
[r^2\partial_r^2 - \ell(\ell + 1)] \Phi_{[\ell'][\ell]}(k, r) \approx 0, \quad r \in [0, \delta].
\]  

(A1)

Each of these equations has two independent solutions behaving as \( \sim r^{\ell+1} \) and \( \sim r^{-\ell} \) and of course the trivial (zero) solution. Therefore a regular column consists only of \( \sim r^{\ell+1} \) and zero elements. Therefore the only way to construct the regular matrix \( \|\Phi(k, r)\| \) obeying Eq. (A1) with linearly independent columns, is to choose its diagonal as follows

\[
\|\Phi(k, r)\| \overset{r \to 0}{\sim} \begin{pmatrix}
  r^{\ell_1+1} & 0 & \cdots & 0 \\
  0 & r^{\ell_2+1} & \cdots & 0 \\
  \vdots & \vdots & \ddots & \vdots \\
  0 & 0 & \cdots & r^{\ell_N+1}
\end{pmatrix}
\]  

(A2)

which obviously satisfies the above-mentioned three properties. Higher order corrections to Eq. (A1) give, of course, non–zero off-diagonal elements. Each column of the matrix (A2) is a solution of Eq. (A2) and therefore has, separately, the short–range behaviour

\[
\begin{pmatrix}
  \Phi_{[\ell_1][\ell_1]}(k, r) \\
  \Phi_{[\ell_2][\ell_1]}(k, r) \\
  \vdots \\
  \Phi_{[\ell_n][\ell_1]}(k, r) \\
  \vdots \\
  \Phi_{[\ell_N][\ell_1]}(k, r)
\end{pmatrix} \overset{r \to 0}{\sim} \begin{pmatrix}
  0 \\
  0 \\
  \vdots \\
  r^{\ell_n+1} \\
  \vdots \\
  0
\end{pmatrix}.
\]  

(A3)
Hence when \( r \to 0 \) all elements of the left hand side column of Eq. \( \text{(A3)} \) with \([\ell] \neq [\ell']\) vanish faster than the one with \([\ell] = [\ell']\). In other words, the off-diagonal elements of a column are infinitesimal as compared to the diagonal one. Therefore we can rewrite Eq. \( \text{(A2)} \) indicating the higher order corrections as follows

\[
\| \Phi(k, r) \| \sim \left( \begin{array}{ccc}
    r^{\ell_1+1} & o(r^{\ell_2+1}) & \cdots & o(r^{\ell_N+1}) \\
    o(r^{\ell_1+1}) & r^{\ell_2+1} & \cdots & o(r^{\ell_N+1}) \\
    \vdots & \vdots & \ddots & \vdots \\
    o(r^{\ell_1+1}) & o(r^{\ell_2+1}) & \cdots & r^{\ell_N+1}
\end{array} \right). \quad \text{(A4)}
\]

The inclusion of the higher order terms retains the linear independence of the columns. Indeed,

\[
\det \| \Phi(k, r) \| = \prod_i r^{\ell_i+1} + o \left( \prod_i r^{\ell_i+1} \right),
\]

because the products involving off-diagonal elements always contain at least one of the factors \( o(r^{\ell_1+1}), o(r^{\ell_2+1}), \cdots, o(r^{\ell_N+1}) \). Hence

\[
\det \| \Phi(k, r) \| \to_{r \to 0} \prod_i r^{\ell_i+1}
\]

and on the interval \((0, \delta]\) we can always find at least one point \( r_0 \) where \( \det \| \Phi(k, r) \| \neq 0 \). This means that the columns of the matrix \( \text{(A4)} \) are linearly independent on the whole interval \((0, \delta]\).

The structure of the matrix \( \text{(A4)} \) implies that the behaviour of the regular basis in the immediate vicinity of the point \( r = 0 \) is such that

\[
\lim_{r \to 0} \frac{\Phi[\ell][\ell'](k, r)}{r^{\ell+1}} = \delta[\ell][\ell'].
\]

Since we can choose the normalisation constant in each element of the matrix \( \| \Phi(k, r) \| \) independently, we may replace \( r^{\ell+1} \) in the last equation by \((kr)^{\ell+1}\) to get the boundary condition in the form

\[
\lim_{r \to 0} \frac{\Phi[\ell][\ell'](k, r)}{j_\ell(kr)} = \delta[\ell][\ell'].
\]

\( \text{(A5)} \)

To obtain the higher order terms of \( \text{(A4)} \) in an explicit form we replace \( \| \Phi(k, r) \| \) by the combination of the two new unknown matrix functions \( F^{(\pm)}(k, r) \), as is given by Eq. \( \text{(15)} \), which are subjected to the constraint \( \text{(16)} \) and obey Eqs. \( \text{(17)} \). Since by definition the matrix \( \| \Phi(k, r) \| \) is regular at \( r = 0 \), we have

\[
h^{(\pm)}(kr) F^{(\pm)}[\ell][\ell'](k, r) \to_{r \to 0} -h^{(-)}(kr) F^{(-)}[\ell][\ell'](k, r).
\]

On the other hand

\[
\frac{h^{(\pm)}(kr)}{h^{(-)}(kr)} \equiv \frac{j_\ell(kr) + in_\ell(kr)}{j_\ell(kr) - in_\ell(kr)} \to_{r \to 0} -1,
\]
from which we conclude that in the immediate vicinity of the point \( r = 0 \) the matrices \( \|F^{(+)}(k, r)\| \) and \( \|F^{(-)}(k, r)\| \) become identical, i. e.,
\[
\|F^{(\pm)}(k, r)\| \xrightarrow{r \to 0} \|A(k, r)\|,
\]
where the matrix \( \|A(k, r)\| \) describes their common short–range asymptotic behaviour. Thus, we obtain
\[
\Phi_{i|j'[0]}(k, r) \xrightarrow{r \to 0} \frac{1}{2} \left[ h^{(+)}_\ell(kr) + h^{(-)}_\ell(kr) \right] A_{i|j'[0]}(k, r) = j_\ell(kr)A_{i|j'[0]}(k, r). \quad \text{(A6)}
\]
Comparing the last two equations with Eq. (A5), we get the following boundary conditions for the matrices \( \|F^{(\pm)}(k, r)\| \)
\[
\lim_{r \to 0} \frac{j_\ell(kr)F^{(\pm)}_{i|j'[0]}(k, r)}{j_{\ell'}(kr)} = \delta_{[0][\epsilon]} . \quad \text{(A7)}
\]
Note that unlike (A5), these conditions do not demand that all elements of the matrices \( \|F^{(\pm)}\| \) be regular. Indeed, when \( \ell > \ell' \) Eq. (A7) holds even if \( F^{(\pm)}_{i|j'[0]}(k, r) \sim r^{-(\ell'-\ell)} \) with any \( \epsilon > 0 \). Hence, the left bottom corners of the matrices \( \|F^{(\pm)}\| \) may, in principle, have diverging elements. As can be seen from the structure of the regular basis, Eq. (5), the functions \( F^{(\pm)}_{i|j'[0]}(k, r) \) are closely related to the Jost solutions and thus their singular behaviour is not surprising. The \( \Phi_{i|j'[0]}(k, r) \) itself remains always regular due to the presence of \( j_\ell(kr) \) in (A6) which compensates the diverging terms.

Eq. (A7) gives us the boundary conditions in explicit form only for the diagonal elements of the matrices \( \|F^{(\pm)}\| \) while for the off-diagonal ones it only implies that \( F^{(\pm)}_{i|j'[0]} \sim o(j_\ell/j_{\ell'}) \).

To obtain them explicitly, let us take indefinite integrals in both sides of Eqs. (A7). This gives
\[
F^{(\pm)}_{i|j'[0]}(k, r) = \text{const} \pm \frac{1}{ik} \int h^{(\pm)}_\ell(kr) \sum_{j''} W_{i|j'[0]}(r) \Phi_{j''|j'[0]}(k, r) dr . \quad \text{(A8)}
\]
The integration constants are fixed for the diagonal and the right–top corner elements by the conditions (A7). Indeed, due to (5) the integrals in (A8) for \( \ell \leq \ell' \) give functions \( (\int r^{-\ell}r^{-2+\varepsilon r^{\ell'+1}} dr, \quad \varepsilon > 0 ) \) which vanish at \( r = 0 \). Hence to fulfil (A7) we must set \( \text{const}=1 \) for \( \ell = \ell' \) and \( \text{const}=0 \) for \( \ell < \ell' \). For the left–bottom elements we still have to choose the normalisation which is fixed by letting \( \text{const} = \delta_{[0][\epsilon]} \). Thus finally
\[
F^{(\pm)}_{i|j'[0]}(k, r) = \delta_{[0][\epsilon]} \pm \frac{1}{ik} \int h^{(\pm)}_\ell(kr) \sum_{j''} W_{i|j'[0]}(r) \Phi_{j''|j'[0]}(k, r) dr , \quad \text{(A9)}
\]
where the indefinite integrals should be understood as primitive functions since all arbitrary constants have been fixed already.

Consider now Eqs. (A5) on a small interval \( r \in (0, \delta] \), where all functions under the integral can be replaced by their power–series expansions. While this is possible for \( h^{(\pm)}_\ell(kr) \) and \( W_{i|j'[0]}(r) \), for \( \Phi_{i|j'[0]}(k, r) \) only the diagonal elements are known,
\[
\Phi_{i|j'[0]}(k, r) \approx j_\ell(kr) , \quad r \in (0, \delta] .
\]
As can be seen from Eq. (A4) the elements of the matrix $\|\Phi\|$ vanish (when $r \to 0$) with different speeds. In particular, in each row this speed increases from left to right. At the same time, within each column the element situated on the matrix diagonal has the lowest vanishing speed. This means that the leading term of the series expansion of a column is a column which is filled with zeros except the diagonal element. Looking at either the differential equations (17) or the integral equations (A9), we see that in fact they are independent equations for each column. The series expansion of $\|\Phi\|$ should therefore be individually constructed for each column. Thus the leading term $\|\Phi^{(0)}\|$ of such an expansion is

$$\Phi^{(0)}_{[\ell][\ell]}(k, r) = j\ell(kr)\delta_{[\ell][\ell]} \quad r \in [0, \delta],$$

which, according to (A6), implies that

$$F^{(\pm)(0)}_{[\ell][\ell]}(k, r) = \delta_{[\ell][\ell]} \quad r \in [0, \delta].$$

Substituting (A10) into the indefinite integral (A9) and using the series expansions of $h_k$, $j\ell$, and $W_{[\ell][\ell]}$, we obtain the first iteration $\|F^{(\pm)}_{(1)}\|$ for all elements of the matrices $\|F^{(\pm)}\|$ and thus we can get $\|\Phi^{(1)}\|$ which includes the next terms of the expansion of the regular solution. Using this iterative procedure we can find as many terms of the expansion as needed by the following recurrence formulae

$$
F^{(\pm)(n+1)}_{[\ell][\ell]}(k, r) = \delta_{[\ell][\ell]} \pm \frac{1}{ik} \int h^{(\mp)}_k(kr) \sum_{[\ell'']} W_{[\ell][\ell'']} (r) \Phi^{(n)}_{[\ell''][\ell']} (k, r) \, dr, \quad (A12)
$$

$$
\Phi^{(n)}_{[\ell][\ell]}(k, r) = \frac{1}{2} \left[ h^{(+)}_k(kr) F^{(+)(n)}_{[\ell][\ell]} (k, r) + h^{(-)}_k(kr) F^{(-)(n)}_{[\ell][\ell]} (k, r) \right]. \quad (A13)
$$

### 2. Behaviour at large distances

To analyse the long-range behaviour of the matrix–functions $\|F^{(\pm)}(k, r)\|$ we rewrite the system (17) as follows

$$\partial_r F^{(\pm)}_{[\ell][\ell]} (k, r) = \pm \frac{1}{ik} h^{(\mp)}_k(kr) \sum_{[\ell'']} W_{[\ell][\ell'']} (r) \Phi^{(n)}_{[\ell''][\ell']} (k, r)$$

It is clear that if the limits $\lim_{r \to \infty} \|F^{(\pm)}(k, r)\|$ exist, then the corresponding derivatives $\partial_r \|F^{(\pm)}(k, r)\|$ are zero at large distances. The converse is valid, however, only if the derivatives vanish faster than $r^{-1}$. Indeed, when the derivative of a function $\varphi(r)$ behaves as

$$\frac{d\varphi(r)}{dr} \sim r^{-(\varepsilon+1)}$$

the asymptotic behaviour of the function itself can be written as

$$\varphi(r) \sim \int r^{-(\varepsilon+1)} dr = \text{const} + \begin{cases} \ln r & \varepsilon = 0 \\ -\frac{1}{\varepsilon r^\varepsilon} & \varepsilon \neq 0 \end{cases}.$$
which obviously has a finite limit only if $\varepsilon > 0$.

Therefore, to establish the domains of the $k$–plane where the limits $\lim_{r \to \infty} \|F^{(\pm)}(k, r)\|$ exist, it is sufficient to find out at which areas of this plane the right–hand sides of Eqs. (A14) vanish at large distances faster than the Coulomb potential. For this we, first of all, need to know how the basic solutions $\Phi_{[\ell][\ell']}(k, r)$ behave in different domains of the $k$–plane when $r \to \infty$. To this end we consider Eqs. (11) at large $r$. If the potential is of short–range (decaying exponentially or faster) these equations are reduced to the un–coupled Riccati–Bessel equations, viz.,

$$
\left[\frac{\partial^2}{\partial r^2} + k^2 - \ell(\ell + 1)/r^2\right] \Phi_{[\ell][\ell']}(k, r) \longrightarrow 0. \tag{A15}
$$

Considering them as one matrix equation, then there are two linearly independent solutions which can be chosen as

$$
\|h^{(\pm)}(kr)\| \equiv \begin{pmatrix}
h^{(\pm)}_{\ell_1}(kr) & 0 & \cdots & 0 \\
0 & h^{(\pm)}_{\ell_2}(kr) & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & h^{(\pm)}_{\ell_N}(kr)
\end{pmatrix}. \tag{A16}
$$

Any other solution is a linear combination of them. Therefore

$$
\|\Phi(k, r)\| \longrightarrow \|h^{(\pm)}(kr)\| \cdot \|C_1\| + \|h^{(-)}(kr)\| \cdot \|C_2\|, \tag{A17}
$$

and according to (24)

$$
\|\Phi(k, r)\| \longrightarrow \exp(ikr)\|\tilde{C}_1\| + \exp(-ikr)\|\tilde{C}_2\|. \tag{A18}
$$

If $\text{Im} kr = 0$ then both terms of the last asymptotic relation are oscillating and therefore the regular solution is bounded, i.e.,

$$
\left|\Phi_{[\ell][\ell']}(k, r)\right| \leq \text{const}, \quad \forall \, \ell, \ell' \quad \text{when} \, \quad r \to \infty. \tag{A19}
$$

For $\text{Im} kr \neq 0$, the regular solution diverges due either to the first or the second term of (A18). In this case we can keep only the diverging term of it, viz.,

$$
\|\Phi(k, r)\| \sim \exp(-ikr)\|\tilde{C}_2\| \quad \text{Im} kr > 0, \tag{A20}
$$

$$
\|\Phi(k, r)\| \sim \exp(+ikr)\|\tilde{C}_1\| \quad \text{Im} kr < 0. \tag{A21}
$$

There are, however, special points $k_0$ on the $k$–plane, called spectral points, where by definition the regular solution contains only the first term of (A17), i.e.,

$$
\|\Phi(k_0, r)\| \overset{\text{def}}{=} \frac{\text{exp}(+ik_0 r)}{r} \|\tilde{C}_1\|. \tag{A22}
$$

Spectral points situated on the positive imaginary axis correspond to bound states, and those situated under the real axis to resonance states.
Though we have derived Eqs. (A19, A20, A21) describing the asymptotic behaviour of the regular basis, under the assumption that the potential is of the short range, they should be valid also for potentials decaying faster than $\sim 1/r$. The general proof, however, requires more sophisticated mathematical methods which are beyond the scope of this article.

Substituting Eqs. (A19), (A20), (A21), and (A22) into (A14) and using the asymptotic form of the Riccati–Hankel functions, Eq. (24), together with the constraint on the long–range behaviour of the potential, Eq. (6), we find that in general the derivatives of $\|F^{(\pm)}(k, r)\|$ vanish rapidly enough in the different domains of the $k$–plane. The only points where both limits $\lim_{r \to \infty} \|F^{(\pm)}(k, r)\|$ exist simultaneously are those with $\text{Im} kr = 0$ and the spectral points with $\text{Im} kr > 0$.

For real $r$ then $\lim_{r \to \infty} \|F^{(\pm)}(k, r)\|$ exists for $\text{Im} k \leq 0$ and at the spectral points which correspond to bound states, while $\lim_{r \to \infty} \|F^{(-)}(k, r)\|$ exists for $\text{Im} k \geq 0$. In this case the dividing line that separates the two domains of the $k$–plane coincides with the real axis. This line can be turned downwards, to expose the resonance spectral points, by rotating $r$ as given by Eq. (27). Indeed, if $\phi$ is the polar angle parametrising a point on the $k$–plane

$$k = |k|e^{i\phi},$$

then by choosing large enough $\theta > 0$ we can make $\text{Im} kr$,

$$\text{Im} kr = \text{Im} \left(\frac{|k|xe^{(\phi+\theta)}}{|x|} \sin(\theta + \phi)\right),$$

(A23)

positive even when $\phi$ is negative, $-\theta \leq \phi \leq \pi - \theta$, i.e., when the point $k$ is in the fourth quadrant. From the last equation is clear that when $\theta \neq 0$ the dividing line is $[-\infty e^{-i\theta}, +\infty e^{-i\theta}]$ (see Fig. [1]).

It is worthwhile to mention that the border separating the two domains of the complex $k$–plane is a line only in the case of long–range potentials obeying the condition (6). If however the potential decays at large $r$ exponentially, then $\lim_{r \to \infty} \|F^{(\pm)}(k, r)\|$ exists also within a band above the dividing line while $\lim_{r \to \infty} \|F^{(-)}(k, r)\|$ in the symmetric band below this line. The faster the potential decays the wider this band is. For example, if the potential decays as $\sim \exp(-\mu r)$ then the right hand side of the second equation of the system (A14) behaves, below the dividing line ($\text{Im} kr < 0$), as

$$\partial_r F^{(-)}(k, r) \sim e^{ikr}e^{-\mu r}e^{ikr} = e^{i(2\text{Re} kr - \mu \text{Im} r)} \exp(-2\text{Im} kr - \mu \text{Re} r).$$

The last exponential function decays at large distances if $\text{Im} kr > -\frac{\mu}{2} \text{Re} r$, i.e., when

$$|k| \sin(\theta + \phi) > -\frac{\mu}{2} \cos \theta.$$

(A24)

If $\theta = 0$, this condition reads $\text{Im} k > -\mu/2$ which enables us to locate also virtual states (spectral points on the negative imaginary axis) situated not far from the origin.
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### TABLE I. Bound states generated by the RSC and Moscow potentials

| potential | $k_0$ (fm$^{-1}$) | $E_0$ (MeV) | $D\%$ | Refs. |
|-----------|------------------|-------------|-------|-------|
| RSC       | 0.2316110        | −2.22460    | 6.470 | –     |
| Moscow    | 3.5571773        | −524.741    | 14.36 | –     |
| Moscow    | 0.2316000        | −2.22439    | 6.588 | –     |

### TABLE II. Jost matrix for the RSC potential at $k = 0.5 \exp(-i0.3\pi)$ fm$^{-1}$, calculated with $x_{\text{max}} = 50$ fm and three different values of the rotation angle $\theta$.

| $\theta$ | $\|F^{-}(k, x_{\text{max}}e^{i\theta})\|$ |
|-----------|---------------------------------|
| 0         | $\begin{pmatrix} 22637458292890 + i14763693403731 & -22818484 + i84501579 \\ 8536691059869 + i6193286881927 & 10532586 + i32492267 \end{pmatrix}$ |
| 0.35$\pi$ | $\begin{pmatrix} -325291222087 + i639117048997 & -2294097 - i362305 \\ 145085673415 - i1488370181212 & 4729536 - i1042674 \end{pmatrix}$ |
| 0.40$\pi$ | $\begin{pmatrix} -325288820471 + i639116901481 & -2294097 - i362305 \\ 145081315229 - i1488368045635 & 4729536 - i1042675 \end{pmatrix}$ |
TABLE III. Spectral points of the model potential (see text) with $\lambda = 15\text{ MeV}$.

| $\text{Re} p_0 (\text{fm}^{-1})$ | $\text{Im} p_0 (\text{fm}^{-1})$ | $E_0$ (MeV) | $\Gamma$ (MeV) |
|-------------------------------|-------------------------------|--------------|--------------|
| 0                             | 4.5581531714                 | −10.3883801672 | 0            |
| 0                             | 4.023079863                  | −8.09258579   | 0            |
| 0                             | 3.471206989                  | −6.02463898   | 0            |
| 0                             | 2.899849780                  | −4.20456437   | 0            |
| 0                             | 2.305427868                  | −2.65749883   | 0            |
| 0                             | 1.681898798                  | −1.41439178   | 0            |
| 0                             | 1.01619035                   | −0.5163214    | 0            |
| 0                             | 0.254097                     | −0.0322826    | 0            |
| 3.44660892                    | −0.53011439                  | 5.79904590    | 3.6541940    |
| 4.1388078309                  | −0.1467148600                | 8.5541025053  | 1.214449223  |
| 4.46521096                    | −0.686071761                 | 9.733790724   | 6.12691030   |
| 4.744324                      | −1.332365                    | 10.36671      | 12.64234     |
| 4.96356                       | −1.99719                     | 10.3241       | 19.8263      |
| 5.1410                        | −2.6634                      | 9.6681        | 27.385       |
FIG. 1. Complex rotation of the coordinate and corresponding domains of the $k$–plane where the limits of the matrices $\| F^{(\pm)}(k, r) \|$ exist.
FIG. 2. Spectral points (filled circles) of the model potential with $\lambda = 15$ MeV. The large open circles represent three of the resonances generated by the central potential $V_c$ and the small circles show the movement of the resonances when $\lambda$ decreases from 15 MeV to zero in steps of $\Delta \lambda = 1$ MeV. The dividing line corresponds to $\theta = 0.2\pi$. 