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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 analytic 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.

1. Introduction

Almost any textbook on the scattering theory has a chapter devoted to the Jost function, but none of them gives a practical method for its calculation; they provide instead equations expressing the Jost function in terms of the wavefunction. However, to use them one must find the wavefunction 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 in which 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 [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 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 uncoupled waves, then the problem of singularity is inevitable and thus one must resort to alternative methods.

In this work, we show that for the class of so-called analytic potentials (which are holomorfic functions of r in the first quadrant of the complex r-plane) 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 have been proposed for bound- and scattering-state calculations, that is for calculations in the upper half of the complex momentum plane [4].

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Exploiting the idea of the complex rotation of the radial coordinate [5], $r \to r\exp(\mathrm{i}\theta)$, 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 wavefunction 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 [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 generalize 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.

This paper is organized as follows. In sections 2 and 3 our formalism is presented, while in section 4 the method is applied to several examples and the results obtained are discussed. Our conclusions are given in section 5. Finally some mathematical details and proofs are given in the appendix.

2. Formalism

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

Since these types of potentials are not rotationally invariant, the angular momentum ℓ associated with the interparticle coordinate $\boldsymbol{r}$, is not conserved. Therefore a partial-wave decomposition of the Schrödinger equation results in a system of coupled equations for states with different ℓ. 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 a few partial waves are coupled to each other, namely, those in which the non-central part of the potential stems from the non-zero spins of the particles involved. In such systems the total angular momentum,

$$\boldsymbol{J} = \boldsymbol{\ell} + \boldsymbol{s}$$

is conserved and the total spin $\boldsymbol{s}$ defines the maximal number of coupled partial waves by the triangle condition

$$|J - s| \leqslant \ell \leqslant |J + s|. \tag{1}$$

We shall consider a problem of this kind though all formulae remain applicable to the more general case of coupled partial waves.

2.1. Partial waves for discrete spectrum

Wavefunctions $\Psi_{kJM}(\boldsymbol{r})$ 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 π which is omitted in our notation. Such wavefunctions can be expanded in terms of the spin-angular functions

$$\mathcal{Y}^{JM}_{[\ell]}(\hat{\boldsymbol{r}}) \equiv \sum_{m\mu} C^{JM}_{\ell m s\mu} Y_{\ell m}(\hat{\boldsymbol{r}})\chi_{s\mu}$$

as

$$\Psi_{kJM}(\boldsymbol{r}) = \frac{1}{r}\sum_{[\ell]} \mathcal{Y}^{JM}_{[\ell]}(\hat{\boldsymbol{r}}) u^{J}_{[\ell]}(k,r) \tag{2}$$

where $u^{J}_{[\ell]}(k,r)$ 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, ℓm instead of ℓs. Furthermore all formulae can be generalized to coupled hyper-radial equations simply by replacing $[\ell]$ by $[L]$ where L is the grand orbital quantum number (for hyper-radial equations [8]). For simplicity we drop the quantum numbers JM where convenient.

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

$$[\partial_r^2 + k^2 - \ell(\ell+1)/r^2] u^{J}_{[\ell]}(k,r) = \sum_{[\ell']} W^{J}_{[\ell][\ell']}(r) u^{J}_{[\ell']}(k,r) \tag{3}$$

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

$$W^{J}_{[\ell][\ell']}(r) \equiv 2m\langle \mathcal{Y}^{JM}_{[\ell]} | V(\boldsymbol{r}) | \mathcal{Y}^{JM}_{[\ell']} \rangle \tag{4}$$

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,

$$\lim_{r\to 0} r^2 W^{J}_{[\ell][\ell']}(r) = 0 \tag{5}$$

and vanish at large distances faster than the Coulomb potential,

$$\lim_{r\to\infty} r W^{J}_{[\ell][\ell']}(r) = 0. \tag{6}$$

2.2. Partial waves for continuum

The scattering-state wavefunction $\Psi_{\boldsymbol{k}s\mu}(\boldsymbol{r})$ is defined by the real vector $\boldsymbol{k}$ (the momentum of the incoming wave), total spin s, and its third component μ. 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 $\boldsymbol{k}$. Since $\Psi_{\boldsymbol{k}s\mu}(\boldsymbol{r})$ depends on the two vectors $\boldsymbol{k}$ and $\boldsymbol{r}$, we have to perform partial-wave analysis in both the momentum and coordinate space[1, 9],

$$\Psi_{\boldsymbol{k}s\mu}(\boldsymbol{r}) = \sqrt{\frac{2}{\pi}}\frac{1}{kr}\sum_{JM[\ell']\ell} \mathcal{Y}^{JM}_{[\ell']}(\hat{\boldsymbol{r}}) u^{J}_{[\ell'][\ell]}(k,r) Y^{JM*}_{[\ell]\mu}(\hat{\boldsymbol{k}}) \tag{7}$$

where

$$Y^{JM}_{[\ell]\mu}(\hat{\boldsymbol{k}}) \equiv \mathrm{i}^{-\ell}\sum_{m} C^{JM}_{\ell m s\mu} Y_{\ell m}(\hat{\boldsymbol{k}})$$

and the radial wavefunction $u^{J}_{[\ell'][\ell]}(k,r)$ obeys the same equation as $u^{J}_{[\ell]}(k,r)$,

$$[\partial_r^2 + k^2 - \ell(\ell+1)/r^2] u^{J}_{[\ell][\ell']}(k,r) = \sum_{[\ell'']} W^{J}_{[\ell][\ell'']}(r) u^{J}_{[\ell''][\ell']}(k,r). \tag{8}$$

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

$$\begin{aligned} u_{[\ell]}(k,r) &\underset{r\to 0}{\longrightarrow} 0 \\ u_{[\ell'][\ell]}(k,r) &\underset{r\to 0}{\longrightarrow} 0 \end{aligned} \tag{9}$$

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

$$\begin{aligned} u_{[\ell]}(k,r) &\underset{r\to \infty}{\longrightarrow} U_{[\ell]}(k,r) \\ u_{[\ell'][\ell]}(k,r) &\underset{r\to \infty}{\longrightarrow} U_{[\ell'][\ell]}(k,r) \end{aligned} \tag{10}$$

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 equation (3) defined only by the condition (9) and not subjected to any restrictions at large r.

2.3. Regular basis

From the wide variety of solutions obeying (9) 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 wavefunctions can be constructed in terms of such a basis.

Let us consider equation (3) as a matrix equation. Then, each of its solutions is a column matrix. From the general theory of differential equations it is known that there are as many independent regular column solutions of equation (3) as the column dimension, i.e. the number of equations in the system. These columns can be combined in a square matrix $\|\Phi_{[\ell][\ell']}\|$ satisfying

$$[\partial_r^2 + k^2 - \ell(\ell+1)/r^2]\Phi_{[\ell][\ell']}(k,r) = \sum_{[\ell'']} W_{[\ell][\ell'']}(r)\Phi_{[\ell''][\ell']}(k,r) \tag{11}$$

with

$$\Phi_{[\ell][\ell']}(k,r) \underset{r\to 0}{\longrightarrow} 0 \qquad \forall[\ell],[\ell']. \tag{12}$$

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

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

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.

As in any other space, the basis can be chosen in an infinite number of ways by specifying the behaviour (12). The possible choice of condition (12), however, is not entirely arbitrary. In [10] it was shown (see also an alternative proof in the appendix) that for potentials fulfilling restriction (5), the regular columns are only linearly independent 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 a condition guarantees the linear independence of the columns since in each row the elements have different behaviours (different powers of r) near $r = 0$. If instead of the rows, we look at the columns, we find from equation (13) that in each of them all off-diagonal elements vanish faster than the diagonal one.

Despite 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 regularization of the integral equation for $\Phi_{[\ell][\ell']}$ [1].

To be consistent with the definition of the regular solution for the uncoupled partial waves [11], we choose the normalization coefficients in such a way that

$$\lim_{r\to 0} \frac{\Phi_{[\ell][\ell']}(k,r)}{j_{\ell'}(kr)} = \delta_{[\ell][\ell']} \tag{14}$$

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 condition (14) only implies that $\Phi_{[\ell][\ell']} \sim \mathrm{o}(j_{\ell'})$, $\ell \neq \ell'$. 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 method for obtaining series expansions (in powers of r) 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 equation (11) into another equivalent form suitable for the construction of different physical solutions. For this we introduce two new unknown matrices $\|F^{(\pm)}_{[\ell][\ell']}(k,r)\|$ and assume the following ansatz for the regular solution

$$\Phi_{[\ell][\ell']}(k,r) = \tfrac{1}{2}[h^{(+)}_\ell(kr) F^{(+)}_{[\ell][\ell']}(k,r) + h^{(-)}_\ell(kr) F^{(-)}_{[\ell][\ell']}(k,r)] \tag{15}$$

where the Riccati–Hankel functions $h^{(\pm)}_\ell$ are linear combinations of the Riccati–Bessel and Riccati–Neumann functions $h^{(\pm)}_\ell(z) \equiv j_\ell(z) \pm \mathrm{i} n_\ell(z)$ [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 $h^{(\pm)}_\ell(kr)$ 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 constraint. The most convenient is the Lagrange condition

$$h^{(+)}_\ell(kr)\partial_r F^{(+)}_{[\ell][\ell']}(k,r) + h^{(-)}_\ell(kr)\partial_r F^{(-)}_{[\ell][\ell']}(k,r) = 0 \tag{16}$$

which is a standard choice in the variable–constant method for solving differential equations [13]. Substituting (15) into equation (11) and using condition (16), we obtain the following first-order coupled differential matrix equations

$$\partial_r F^{(\pm)}_{[\ell][\ell']}(k,r) = \pm \frac{h^{(\mp)}_\ell(kr)}{2\mathrm{i}k} \sum_{[\ell'']} W_{[\ell][\ell'']}(r)\{h^{(+)}_{\ell''}(kr) F^{(+)}_{[\ell''][\ell']}(k,r) + h^{(-)}_{\ell''}(kr) F^{(-)}_{[\ell''][\ell']}(k,r)\}. \tag{17}$$

As we show in the appendix, the boundary condition (14) can be rewritten as

$$\lim_{r\to 0}\left[\frac{j_\ell(kr)F^{(\pm)}_{[\ell][\ell']}(k,r)}{j_{\ell'}(kr)}\right]=\delta_{[\ell][\ell']} \tag{18}$$

and a series expansion for $\|F^{(\pm)}_{[\ell][\ell']}(k,r)\|$ in powers of r near the point $r=0$ can be found iteratively as follows. Starting from the unit matrices

$$F^{(\pm)(0)}_{[\ell][\ell']}(k,r)=\delta_{[\ell][\ell']} \tag{19}$$

we obtain all the subsequent iterations for $\|F^{(\pm)}\|$ by evaluating the indefinite integrals (the primitive functions)

$$F^{(\pm)(n+1)}_{[\ell][\ell']}(k,r)=\delta_{[\ell][\ell']}\pm\frac{1}{2\mathrm{i}k}\int h^{(\mp)}_\ell(kr)\sum_{[\ell'']}W_{[\ell][\ell'']}(r)$$
$$\times[h^{(+)}_{\ell''}(kr)F^{(+)(n)}_{[\ell][\ell']}(k,r)+h^{(-)}_{\ell''}(kr)F^{(-)(n)}_{[\ell][\ell']}(k,r)]\,\mathrm{d}r \tag{20}$$

where $h^{(\mp)}_\ell(kr)$ and $W_{[\ell][\ell'']}(r)$ are replaced by their r-power series expansions and the arbitrary constants of the integration are zero. We shall give an explicit example for this expansion in section 4.

In contrast to equation (11), 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 (5) the potential may also behave near this point as $\sim r^{-(2-\varepsilon)}$, $\varepsilon>0$. Therefore equations (17) cannot be solved numerically 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 $r=\delta$ as

$$F^{(\pm)}_{[\ell][\ell']}(k,\delta)\approx F^{(\pm)(N)}_{[\ell][\ell']}(k,\delta). \tag{21}$$

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 emphasized that although certain elements of $\|F^{(\pm)}\|$ diverge, the matrix $\|\Phi\|$ must always, by definition, be regular. This can also be seen from the fact that the boundary conditions (18) follow from the regular boundary conditions (14). Therefore the singularities of the two terms of the ansatz (15) should cancel out. As shown in the appendix, this is indeed the case. The system of equations (17) together with the boundary values (21) represent a well-defined differential problem, a solution of which gives the regular basis in the form (15).

2.4. Jost matrices

It can be proved (see the appendix) that for $\mathrm{Im}\,k=0$ the right-hand side of equations (17) vanishes when $r\to\infty$. Since the corresponding derivatives also vanish, the functions $F^{(\pm)}_{[\ell][\ell']}(k,r)$ become r-independent and thus, for momenta corresponding to the scattering states, we have

$$\Phi_{[\ell][\ell']}(k,r)\underset{r\to\infty}{\longrightarrow}\tfrac{1}{2}[h^{(+)}_\ell(kr)\mathcal{F}^{(+)}_{[\ell][\ell']}(k)+h^{(-)}_\ell(kr)\mathcal{F}^{(-)}_{[\ell][\ell']}(k)] \tag{22}$$

where

$$\mathcal{F}^{(\pm)}_{[\ell][\ell']}(k)=\lim_{r\to\infty}F^{(\pm)}_{[\ell][\ell']}(k,r). \tag{23}$$

We may call these r-independent matrices $\|\mathcal{F}^{(\pm)}\|$ *Jost matrices*. The products

$$h_\ell^{(\pm)}(kr)\sum_{[\ell'']}\|F^{(\pm)}_{[\ell][\ell'']}(k,r)\|\cdot\|\mathcal{F}^{(\pm)}_{[\ell''][\ell']}(k)\|^{-1} \tag{24}$$

which behave asymptotically like $\sim \mathrm{e}^{\pm \mathrm{i}kr}$, in this respect are similar to the commonly used *Jost solutions*.

In the context of coupled partial waves the Jost solutions of equation (11) may be defined as matrix functions given by equation (15) in terms of $F^{(\pm)}$ which obey equations (17) with the boundary conditions

$$F^{(+)}_{[\ell][\ell']}(k,r)\underset{r\to\infty}{\longrightarrow}\begin{cases}2 & \text{solution I}\\ 0 & \text{solution II}\end{cases}\qquad F^{(-)}_{[\ell][\ell']}(k,r)\underset{r\to\infty}{\longrightarrow}\begin{cases}0 & \text{solution I}\\ 2 & \text{solution II.}\end{cases} \tag{25}$$

Then at large distances the regular solution, which is a linear combination of the two Jost solutions, consists of two terms of the type (24). Practically the Jost solutions can be obtained by solving equations (17) inwards starting at a sufficiently large r with the boundary values (25).

For complex values of k the limits (23) generally exist in different domains of the complex k-plane, namely, $\mathcal{F}^{(+)}_{[\ell][\ell']}(k)$ in the lower half ($\mathrm{Im}\,k\leqslant 0$) while $\mathcal{F}^{(-)}_{[\ell][\ell']}(k)$ in the upper half ($\mathrm{Im}\,k\geqslant 0$). This is because, according to equations (17), the derivatives $\partial_r F^{(\pm)}(k,r)$ are proportional to $h_\ell^{(\mp)}(kr)$ with

$$h_\ell^{(\pm)}(kr)\underset{r\to\infty}{\longrightarrow}\mp\mathrm{i}\exp[\pm\mathrm{i}(kr-\ell\pi/2)] \tag{26}$$

vanishing in different domains of the k-plane, namely,

$$h_\ell^{(+)}(kr)\underset{r\to\infty}{\longrightarrow}0\qquad \mathrm{Im}\,(kr)>0 \tag{27}$$

$$h_\ell^{(-)}(kr)\underset{r\to\infty}{\longrightarrow}0\qquad \mathrm{Im}\,(kr)<0. \tag{28}$$

Thus, in general, the only area where the limits (23) simultaneously exist is the real axis†. However, for a particular class of short-range potentials (decaying exponentially or faster) the upper bound for the existence of $\mathcal{F}^{(+)}$ is shifted upwards and the lower bound for $\mathcal{F}^{(-)}$ 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 [6, 7]. Indeed, conditions (27) and (28) involve the imaginary part of the product kr and not of the momentum alone. Therefore, if, for example, $\mathrm{Im}\,(kr)$ is negative we can make it positive by using the complex rotation method which we describe next.

2.5. Complex rotation

In this method the radius r is replaced by a complex one, namely

$$r=x\exp(\mathrm{i}\theta)\qquad x\geqslant 0\qquad 0\leqslant|\theta|<\frac{\pi}{2}. \tag{29}$$

The idea of complex rotation of the coordinate is not new. During World War II, Hartree and co-workers at Manchester University used such a rotation to solve certain differential equations describing radio-wave propagation in the atmosphere (for more details see [14]). Nowadays the complex rotation is widely used for locating quantum resonances

† It can also be proved that both of these limits exist at all spectral points k_0 with $\mathrm{Im}\,k_0 r\geqslant 0$ (see the appendix).

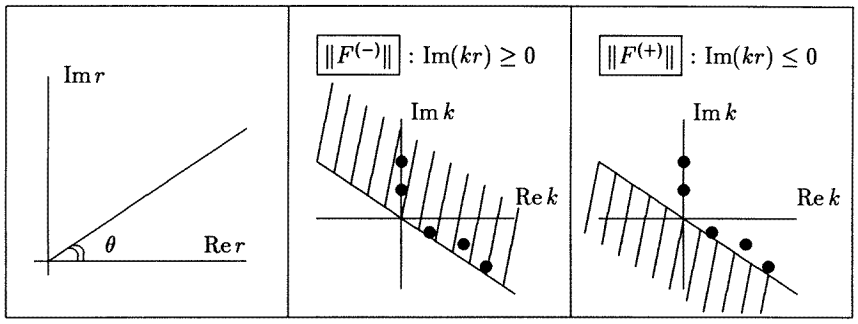

Figure 1. Complex rotation of the coordinate and corresponding domains of the k-plane where the limits of the matrices $\|F^{(\pm)}(k,r)\|$ exist.

by variational methods [5]. In contrast, our equations together with the complex rotation can be used to locate resonances in an exact way.

Applying the complex transformation (29) to equations (17), we obtain

$$\partial_x F^{(\pm)}_{[\ell][\ell']}(k, x\mathrm{e}^{\mathrm{i}\theta}) = \pm\frac{\mathrm{e}^{\mathrm{i}\theta} h^{(\mp)}_{\ell}(kx\mathrm{e}^{\mathrm{i}\theta})}{2\mathrm{i}k} \sum_{[\ell'']} W_{[\ell][\ell'']}(x\mathrm{e}^{\mathrm{i}\theta}) \times\{h^{(+)}_{\ell''}(kx\mathrm{e}^{\mathrm{i}\theta}) F^{(+)}_{[\ell''][\ell']}(k, x\mathrm{e}^{\mathrm{i}\theta}) + h^{(-)}_{\ell''}(kx\mathrm{e}^{\mathrm{i}\theta}) F^{(-)}_{[\ell''][\ell']}(k, x\mathrm{e}^{\mathrm{i}\theta})\}. \tag{30}$$

The purpose of the rotation (29) is to make the imaginary part of the product kr positive or negative, in calculating $\mathcal{F}^{(-)}$ or $\mathcal{F}^{(+)}$ respectively, at points on the k-plane we are interested in. Thus we have $\mathrm{Im}\, kr > 0$ for all points above the dividing line shown in figure 1. This line defined by the negative angle θ in the k-plane results from the rotation (29) in the r-plane with positive θ.

If the potential matrix $\|W(r)\|$ is an analytic function of the complex variable r and obeys the conditions (5) and (6) along the ray (29), then the limit

$$\lim_{x\to\infty} F^{(-)}_{[\ell][\ell']}(k, x\mathrm{e}^{\mathrm{i}\theta}) = \mathcal{F}^{(-)}_{[\ell][\ell']}(k) \tag{31}$$

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

$$\lim_{x\to\infty} F^{(+)}_{[\ell][\ell']}(k, x\mathrm{e}^{\mathrm{i}\theta}) = \mathcal{F}^{(+)}_{[\ell][\ell']}(k) \tag{32}$$

exists and is finite for all k on and below the dividing line. Moreover, when the limits (31) and (32) exist the values of $\mathcal{F}^{(\pm)}_{[\ell][\ell']}(k)$ are independent of the rotation angle θ as the Jost function is r-independent and hence θ-independent. To calculate the $\mathcal{F}^{(-)}_{[\ell][\ell']}(k)$ for $\mathrm{Im}\, k < 0$ we need to solve equation (30) at a sufficiently large positive θ, and the $\mathcal{F}^{(+)}_{[\ell][\ell']}(k)$ for $\mathrm{Im}\, k > 0$ at a sufficiently large negative θ.

2.6. Cancellation of the singularities

We note that although the ansatz (15) is suitable for large distances (see the next section), it is not good for numerical calculations in the vicinity of $r = 0$. Indeed, near this point the matrices $\|F^{(+)}(k,r)\|$ and $\|F^{(-)}(k,r)\|$ become identical and the singularities of $h^{(+)}_{\ell}(kr)$ and $h^{(-)}_{\ell}(kr)$ are cancelled. Although this does not formally cause any problem, in numerical calculations the cancellation of singularities is always a source of possible numerical errors.

These errors increase with increasing ℓ since in this case $h_\ell^{(\pm)}(kr)$ becomes more singular. Therefore, for larger ℓ the point $r = \delta$ must be shifted further from the origin. This in turn, requires more iterations of equation (20) to obtain the boundary values $F_{\ell\ell'}^{(\pm)}(k, \delta)$ to a required accuracy.

There is another way to numerically handle the boundary condition problem. Since

$$\tfrac{1}{2}(h_\ell^+ + h_\ell^-) = j_\ell \qquad \text{and} \qquad \frac{1}{2\mathrm{i}}(h_\ell^+ - h_\ell^-) = n_\ell$$

we may introduce a new pair of matrices

$$\begin{aligned} A_{[\ell][\ell']}(k, r) &\equiv \tfrac{1}{2}[F_{[\ell][\ell']}^{(+)}(k, r) + F_{[\ell][\ell']}^{(-)}(k, r)] \\ B_{[\ell][\ell']}(k, r) &\equiv \frac{1}{2\mathrm{i}}[F_{[\ell][\ell']}^{(+)}(k, r) - F_{[\ell][\ell']}^{(-)}(k, r)] \end{aligned} \tag{33}$$

which transforms the ansatz (15) into the form

$$\Phi_{[\ell][\ell']}(k, r) = j_\ell(kr) A_{[\ell][\ell']}(k, r) - n_\ell(kr) B_{[\ell][\ell']}(k, r) \tag{34}$$

and the corresponding linear combination of equations (17) gives the alternative form

$$\begin{cases} \partial_r A_{[\ell][\ell']}(k, r) = -\dfrac{n_\ell(kr)}{k} \displaystyle\sum_{[\ell'']} W_{[\ell][\ell'']}(r)[j_{\ell''}(kr) A_{[\ell''][\ell']}(k, r) - n_{\ell''}(kr) B_{[\ell''][\ell']}(k, r)] \\ \partial_r B_{[\ell][\ell']}(k, r) = -\dfrac{j_\ell(kr)}{k} \displaystyle\sum_{[\ell'']} W_{[\ell][\ell'']}(r)[j_{\ell''}(kr) A_{[\ell''][\ell']}(k, r) - n_{\ell''}(kr) B_{[\ell''][\ell']}(k, r)]. \end{cases} \tag{35}$$

Likewise, the iterative procedure (19), (20) transforms into

$$A_{[\ell][\ell']}^{(0)}(k, r) = \delta_{[\ell][\ell']} \qquad B_{[\ell][\ell']}^{(0)}(k, r) = 0 \tag{36}$$

$$\begin{cases} A_{[\ell][\ell']}^{(n+1)}(k, r) = \delta_{[\ell][\ell']} - \dfrac{1}{k} \displaystyle\int n_\ell(kr) \sum_{[\ell'']} W_{[\ell][\ell'']}(r)[j_{\ell''}(kr) A_{[\ell''][\ell']}^{(n)}(k, r) \\ \qquad\qquad - n_{\ell''}(kr) B_{[\ell''][\ell']}^{(n)}(k, r)]\, \mathrm{d}r \\ B_{[\ell][\ell']}^{(n+1)}(k, r) = -\dfrac{1}{k} \displaystyle\int j_\ell(kr) \sum_{[\ell'']} W_{[\ell][\ell'']}(r)[j_{\ell''}(kr) A_{[\ell''][\ell']}^{(n)}(k, r) \\ \qquad\qquad - n_{\ell''}(kr) B_{[\ell''][\ell']}^{(n)}(k, r)]\, \mathrm{d}r. \end{cases} \tag{37}$$

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 equations (35) from the boundary values $A_{[\ell][\ell']}(k, \delta)$, $B_{[\ell][\ell']}(k, \delta)$ and at some intermediate point r_{int} (far enough from the origin) to go over to equations (17) with starting values $F_{[\ell][\ell']}^{(\pm)}(k, r_{\mathrm{int}})$ obtained from $A_{[\ell][\ell']}(k, r_{\mathrm{int}})$ and $B_{[\ell][\ell']}(k, r_{\mathrm{int}})$ via the linear combinations (33).

One may argue that we can abandon equations (17) altogether and integrate equation (35) on the whole interval $[\delta, r_{\max}]$ instead. However, $\|F^{(+)}(k, r)\|$ and $\|F^{(-)}(k, r)\|$ 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. 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 equations (35) and finish at large $r_{\max}$ with equations (17).

3. Physical solutions

In the following 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,

$$\begin{aligned} u_{[\ell]}(k,r) &= \sum_{[\ell']} \Phi_{[\ell][\ell']}(k,r)c_{[\ell']} \\ u_{[\ell'][\ell]}(k,r) &= \sum_{[\ell'']} \Phi_{[\ell'][\ell'']}(k,r)c_{[\ell''][\ell]} \end{aligned} \tag{38}$$

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

3.1. Bound states

The bound-state wavefunction vanishes at large distances as

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

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

$$\tfrac{1}{2}\sum_{[\ell']}[h_\ell^{(+)}(kr)\mathcal{F}^{(+)}_{[\ell][\ell']}(k) + h_\ell^{(-)}(kr)\mathcal{F}^{(-)}_{[\ell][\ell']}(k)]c_{[\ell']} \underset{r\to\infty}{\longrightarrow} 0. \tag{39}$$

For bound states $\mathrm{Im}\,k > 0$ and the Riccati–Hankel function $h_\ell^{(+)}(kr)$ decays exponentially while $h_\ell^{(-)}(kr)$ grows exponentially. Therefore condition (39) can only be fulfilled if we find coefficients $c_{[\ell]}$ such that the diverging functions $h_\ell^{(-)}(kr)$ of different columns cancel out, that is, if

$$\sum_{[\ell']} \mathcal{F}^{(-)}_{[\ell][\ell']}(k)c_{[\ell']} = 0. \tag{40}$$

This system of homogeneous linear equations has a non-trivial solution if and only if

$$\det\|\mathcal{F}^{(-)}(k)\| = 0. \tag{41}$$

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 figure 1). For each zero k_0 thus found, the coefficients $c_{[\ell]}$ are then uniquely determined by the system (40) apart from a general normalization factor which is finally fixed when the physical wavefunction,

$$\Psi_{k_0 JM}(\boldsymbol{r}) = \frac{1}{2r}\sum_{[\ell][\ell']} \mathcal{Y}^{JM}_{[\ell]}(\hat{\boldsymbol{r}})[h_\ell^{(+)}(k_0r)F^{(+)}_{[\ell][\ell']}(k_0,r) + h_\ell^{(-)}(k_0r)F^{(-)}_{[\ell][\ell']}(k_0,r)]c_{[\ell']} \tag{42}$$

is normalized. The contribution of each element of the column

$$u_{[\ell]}(k_0,r) = \tfrac{1}{2}\sum_{[\ell']}[h_\ell^{(+)}(k_0r)F^{(+)}_{[\ell][\ell']}(k_0,r) + h_\ell^{(-)}(k_0r)F^{(-)}_{[\ell][\ell']}(k_0,r)]c_{[\ell']} \tag{43}$$

into the normalization integral represents what is usually called the percentage of the corresponding partial wave.

3.2. Scattering states

The scattering states normalized to the δ-function,

$$\langle \Psi_{\boldsymbol{k}s\mu} | \Psi_{\boldsymbol{k}'s'\mu'} \rangle = \delta(\boldsymbol{k} - \boldsymbol{k}')\delta_{ss'}\delta_{\mu\mu'}$$

are defined by the following asymptotic condition

$$\Psi_{\boldsymbol{k}s\mu}(\boldsymbol{r}) \underset{r\to\infty}{\longrightarrow} \frac{1}{(2\pi)^{3/2}}\left[\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}\chi_{s\mu} + \frac{\mathrm{e}^{\mathrm{i}kr}}{r}\sum_{s'\mu'} f_{s'\mu's\mu}\left(k\frac{\boldsymbol{r}}{r}, \boldsymbol{k}\right)\chi_{s'\mu'}\right] \tag{44}$$

where $f_{s'\mu's\mu}(\boldsymbol{k}', \boldsymbol{k})$ is the scattering amplitude. The partial wave decomposition of equation (44) gives for the boundary condition (10) (see [1])

$$u_{[\ell'][\ell]}(k, r) \underset{r\to\infty}{\longrightarrow} \tfrac{1}{2}[h^{(-)}_{\ell'}(kr)\delta_{[\ell'][\ell]} + h^{(+)}_{\ell'}(kr)S^J_{[\ell'][\ell]}(k)]. \tag{45}$$

Therefore the choice of our ansatz (15) for the regular basis is natural and suitable not only for constructing the bound states but the scattering states as well. Indeed, comparing (45) with (22) we find that the coefficients $c_{[\ell'][\ell]}$ in (38) should be chosen as

$$c_{[\ell'][\ell]} = \|\mathcal{F}^{(-)}_{[\ell'][\ell]}(k)\|^{-1}$$

which gives us the S-matrix in the form

$$\|S(k)\| = \|\mathcal{F}^{(+)}(k)\| \cdot \|\mathcal{F}^{(-)}(k)\|^{-1}. \tag{46}$$

Thus, the normalized scattering wavefunction can be constructed from the regular basis as follows

$$\Psi_{\boldsymbol{k}s\mu}(\boldsymbol{r})\frac{1}{\sqrt{2\pi}kr}\sum_{JM\ell}\sum_{[\ell']}\sum_{[\ell'']}\mathcal{Y}^{JM}_{[\ell']}(\hat{\boldsymbol{r}})Y^{JM*}_{[\ell]\mu}(\hat{\boldsymbol{k}})\{h^{(+)}_{\ell'}(kr)F^{(+)}_{[\ell'][\ell'']}(k, r) + h^{(-)}_{\ell'}(kr)F^{(-)}_{[\ell'][\ell'']}(k, r)\}\|\mathcal{F}^{(-)}_{[\ell''][\ell]}(k)\|^{-1}. \tag{47}$$

The scattering phase shifts together with the mixing parameters can be found from the S-matrix given by equation (46).

3.3. Resonances

The resonance (or Siegert) states are described by wavefunctions which at large distances only have outgoing spherical waves

$$\Psi_{kJM}(\boldsymbol{r}) = \frac{1}{r}\sum_{[\ell]}\mathcal{Y}^{JM}_{[\ell]}(\hat{\boldsymbol{r}})u^J_{[\ell]}(k, r) \underset{r\to\infty}{\longrightarrow} \sim \frac{\mathrm{e}^{\mathrm{i}kr}}{r}. \tag{48}$$

More precisely, the resonant boundary condition at large r is

$$u^J_{[\ell]}(k, r) \underset{r\to\infty}{\longrightarrow} N^J_{[\ell]}(k)h^{(+)}_{\ell}(kr) \tag{49}$$

where $N^J_{[\ell]}(k)$ are the partial-wave normalization constants. Since there is not a generally accepted convention about the normalization of Siegert states, the $N^J_{[\ell]}(k)$ may involve an arbitrary coefficient. Solutions of the Schrödinger equation, with the long-range behaviour (49), may exist only at discrete points of the complex k-plane, situated below the real axis (see figure 1). The corresponding radial wavefunctions are regular at the origin and are therefore linear combinations of the regular basis

$$u_{[\ell]}(k, r) = \tfrac{1}{2}\sum_{[\ell']}\{h^{(+)}_{\ell}(kr)F^{(+)}_{[\ell][\ell']}(k, r) + h^{(-)}_{\ell}(kr)F^{(-)}_{[\ell][\ell']}(k, r)\}c_{[\ell']}. \tag{50}$$

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

$$\lim_{r\to\infty}\sum_{[\ell']} F^{(-)}_{[\ell][\ell']}(k, x\mathrm{e}^{\mathrm{i}\theta})c_{[\ell']} = 0 \qquad \theta > 0 \tag{51}$$

which means that $u_{[\ell]}(k,r)$ is expressed only in terms of $h^{(+)}_{\ell}(k,r)$ at large distances. Since θ can be chosen such that $\mathrm{Im}\, kr > 0$, 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 (49) 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 equation (41), and its (rotated) wavefunction by equation (42) where r is now complex.

Since this wavefunction is square integrable we can normalize it to unity and thus the normalization constants $N^J_{[\ell]}$ in (49) can be fixed in a natural way. Therefore the proposed method enables us not only to locate the position of the resonances as zeros of the Jost matrix determinant but also to obtain the correct normalization constants $N^J_{[\ell]}$. In order to obtain physical (unrotated) Siegert wave functions, the Schrödinger equation must be integrated along real r inwards using the boundary condition (49), the found momentum k_0 and normalization constants. This integration will automatically provide a wavefunction which is zero at $r = 0$ because k_0 is a spectral point.

4. 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 [15]), and thus the sum over $[\ell]$ is reduced to $\sum_\ell$. The triplet NN potential can couple 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

$$V(\boldsymbol{r}) = V_c(r) + V_t(r)S_{12} + V_{\ell s}(r)(\boldsymbol{\ell}\cdot\boldsymbol{s}) \tag{52}$$

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

$$S_{12} = \frac{3}{r^2}(\boldsymbol{\sigma}_1\cdot\boldsymbol{r})(\boldsymbol{\sigma}_2\cdot\boldsymbol{r}) - (\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)$$

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

$$\begin{pmatrix} W_{00} & W_{02} \\ W_{20} & W_{22} \end{pmatrix} \equiv 2m \begin{pmatrix} V_c & 2\sqrt{2}V_t \\ 2\sqrt{2}V_t & V_c - 2V_t - 3V_{\ell s} \end{pmatrix} \tag{53}$$

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

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

$$W_{\ell\ell'}(r) \underset{r\to 0}{\longrightarrow} a_{\ell\ell'}r^{-1} + b_{\ell\ell'} + c_{\ell\ell'}r + \cdots \tag{54}$$

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

Using (54) we can obtain the corresponding expansions for $A_{\ell\ell'}(k,r)$ and $B_{\ell\ell'}(k,r)$ via the iterative procedure (36), (37) which are needed to impose the boundary conditions $A_{\ell\ell'}(k,\delta)$ and $B_{\ell\ell'}(k,\delta)$ at a small δ. 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 (37) by their series expansions [12]

$$j_0(kr) = kr - \frac{(kr)^3}{6} + \frac{(kr)^5}{120} - \cdots$$
$$j_2(kr) = \frac{(kr)^3}{15} - \frac{(kr)^5}{210} + \frac{(kr)^7}{7560} - \cdots$$
$$n_0(kr) = -1 + \frac{(kr)^2}{2} - \frac{(kr)^4}{24} + \cdots$$
$$n_2(kr) = -\frac{3}{(kr)^2} - \frac{1}{2} - \frac{(kr)^2}{8} - \cdots.$$

Substituting (36) into (37) and performing the integrations over r for each element of the matrices $\|A\|$ and $\|B\|$ we obtain

$$\|A^{(1)}(k,r)\| = \begin{pmatrix} 1 + a_{00}r & \dfrac{a_{02}k^2}{45}r^3 \\ -\dfrac{3a_{20}}{k^2}r^{-1} & 1 + \dfrac{a_{22}}{5}r \end{pmatrix} \qquad \|B^{(1)}(k,r)\| = \begin{pmatrix} -\dfrac{a_{00}k}{2}r^2 & -\dfrac{a_{02}k^3}{60}r^4 \\ -\dfrac{a_{20}k^3}{60}r^4 & -\dfrac{a_{22}k^5}{1350}r^6 \end{pmatrix}$$

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

$$\|A^{(2)}(k,r)\| = \begin{pmatrix} 1 + a_{00}r + \dfrac{\zeta_{00}}{2}r^2 & \dfrac{a_{02}k^2}{45}r^3 + \dfrac{k^2\zeta_{02}}{60}r^4 \\ -\dfrac{3a_{20}}{k^2}r^{-1} + \dfrac{3\zeta_{20}}{k^2}\ln r & 1 + \dfrac{a_{22}}{5}r + \dfrac{\zeta_{22}}{10}r^2 \end{pmatrix}$$
$$\|B^{(2)}(k,r)\| = \begin{pmatrix} -\dfrac{a_{00}k}{2}r^2 - \dfrac{k\zeta_{00}}{3}r^3 & -\dfrac{a_{02}k^3}{60}r^4 - \dfrac{k^3\zeta_{02}}{75}r^5 \\ -\dfrac{a_{20}k^3}{60}r^4 - \dfrac{k^3\zeta_{20}}{75}r^5 & -\dfrac{a_{22}k^5}{1350}r^6 - \dfrac{k^5\zeta_{22}}{1575}r^7 \end{pmatrix}$$

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

$$\begin{pmatrix} \zeta_{00} & \zeta_{02} \\ \zeta_{20} & \zeta_{22} \end{pmatrix} = \begin{pmatrix} \dfrac{a_{00}^2}{2} + b_{00} - \dfrac{a_{02}a_{20}}{4} & \dfrac{a_{00}a_{02}}{12} + b_{02} + \dfrac{a_{02}a_{22}}{6} \\ \dfrac{a_{20}a_{00}}{2} + b_{20} - \dfrac{a_{22}a_{20}}{4} & \dfrac{a_{20}a_{02}}{12} + b_{22} + \dfrac{a_{22}^2}{6} \end{pmatrix}.$$

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 we have $\|B\| = o(\|A\|)$ for all matrix elements, the second term in the linear combinations $\|F^{(\pm)}\| = \|A\| \pm i\|B\|$ vanishes faster than the first one as $r \to 0$.

The singularities of the matrix $\|A_{[\ell][\ell']}(k,r)\|$ 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 $\|F^{(\pm)}_{[\ell][\ell']}(k,r)\|$ with $\ell > \ell'$ are always singular at $r = 0$

if the potential is non-zero at that point. Nevertheless the functions $\Phi_{[\ell][\ell']}(k,r)$ always remain regular because in equation (34) the singularity of $A_{[\ell][\ell']}(k,r)$ is compensated for by $j_\ell(kr)$. In our case we have

$$\|\Phi\| = \begin{pmatrix} j_0 & 0 \\ 0 & j_2 \end{pmatrix} \begin{pmatrix} A_{00} & A_{02} \\ A_{20} & A_{22} \end{pmatrix} - \begin{pmatrix} n_0 & 0 \\ 0 & n_2 \end{pmatrix} \begin{pmatrix} B_{00} & B_{02} \\ B_{20} & B_{22} \end{pmatrix} \tag{55}$$

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 equation (55) we obtain

$$\|\Phi(k,r)\| \underset{r\to 0}{\longrightarrow} \begin{pmatrix} kr + \frac{a_{00}k}{2}r^2 + \frac{\zeta_{00}k}{6}r^3 + \mathcal{O}(r^4\ln r) & \frac{a_{02}k^3}{180}r^4 + \frac{\zeta_{02}k^3}{300}r^5 + \mathcal{O}(r^6) \\ -\frac{a_{20}k}{4}r^2 + \frac{\zeta_{20}k}{5}r^3\ln r - \frac{\zeta_{20}k}{25}r^3 + \mathcal{O}(r^4\ln r) & \frac{k^3}{15}r^3 + \frac{a_{22}k^3}{90}r^4 + \frac{\zeta_{22}k^3}{210}r^5 + \mathcal{O}(r^6) \end{pmatrix} \tag{56}$$

which explicitly demonstrates that our regular basis obeys the boundary condition (14) and, as mentioned in section 2, 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. In view of the off-diagonal elements, 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 of the potential.

Using a quite different approach, Palumbo [10] derived recurrence formulae for directly constructing the series expansion of the regular basis for the potentials of the type (54). Having performed few iterations of Palumbo's formulae, we found that they generate the same terms as those in equation (56). This is yet another confirmation that our iterative procedures (19), (20) and (36), (37) are correct.

In order to test the proposed method numerically, we choose two different NN potentials of the type (54). The first one is the Reid soft-core (RSC) potential [16], which for $J=1$, $s=1$, $\pi=+1$ has the following form

$$\begin{aligned} V_c(r) &= h_0\frac{\mathrm{e}^{-\alpha r}}{\alpha r} + h_1\frac{\mathrm{e}^{-2\alpha r}}{\alpha r} + h_2\frac{\mathrm{e}^{-4\alpha r}}{\alpha r} + h_3\frac{\mathrm{e}^{-6\alpha r}}{\alpha r} \\ V_t(r) &= h_0\left\{\left[\frac{1}{\alpha r} + \frac{3}{(\alpha r)^2} + \frac{3}{(\alpha r)^3}\right]\mathrm{e}^{-\alpha r} - \left[\frac{12}{(\alpha r)^2} + \frac{3}{(\alpha r)^3}\right]\mathrm{e}^{-4\alpha r}\right\} \\ &\quad + h_4\frac{\mathrm{e}^{-4\alpha r}}{\alpha r} + h_5\frac{\mathrm{e}^{-6\alpha r}}{\alpha r} \\ V_{\ell s}(r) &= h_6\frac{\mathrm{e}^{-4\alpha r}}{\alpha r} + h_7\frac{\mathrm{e}^{-6\alpha r}}{\alpha r} \end{aligned} \tag{57}$$

with

$$\begin{aligned} &h_0 = -10.463\ \text{MeV} \qquad h_1 = 105.468\ \text{MeV} \qquad h_2 = -3187.8\ \text{MeV} \\ &h_3 = 9924.3\ \text{MeV} \qquad h_4 = 351.77\ \text{MeV} \qquad h_5 = -1673.5\ \text{MeV} \\ &h_6 = 708.91\ \text{MeV} \qquad h_7 = -2713.1\ \text{MeV} \qquad \alpha = 0.7\ \text{fm}^{-1}. \end{aligned}$$

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

$$\begin{aligned} V_c(r) &= V_1\mathrm{e}^{-\eta r^2} + V_2(1-\mathrm{e}^{-\gamma r})\frac{\mathrm{e}^{-\beta r}}{\beta r} \\ V_t(r) &= V_2\left[1 + \frac{3}{\beta r} + \frac{3}{(\beta r)^2}\right](1-\mathrm{e}^{-\gamma r})^3\frac{\mathrm{e}^{-\beta r}}{\beta r} \\ V_{\ell s}(r) &\equiv 0 \end{aligned} \tag{58}$$

Table 1. Bound states generated by the RSC and Moscow potentials.

	Our method			[16–18]	
Potential	k_0 (fm^{-1})	E_0 (MeV)	D%	E_0 (MeV)	D%
RSC	i0.231 6110	−2.224 60	6.470	−2.224 60	6.470
Moscow	i3.557 1773	−524.741	14.36	−524.8	—
Moscow	i0.231 6000	−2.224 39	6.588	−2.224 6	6.778

with

$$V_1 = -466.74 \text{ MeV} \qquad V_2 = -10.69 \text{ MeV}$$
$$\beta = 0.6995 \text{ fm}^{-1} \qquad \gamma = 3 \text{ fm}^{-1} \qquad \eta = 1.6 \text{ fm}^{-2}.$$

The RSC potential has a strong repulsion at small distances,

$$\|a_{\ell\ell'}\| = \frac{2m}{\alpha}\begin{pmatrix} h_0+h_1+h_2+h_3 & 2\sqrt{2}(h_4+h_5+23.5h_0) \\ 2\sqrt{2}(h_4+h_5+23.5h_0) & h_1+h_2+h_3-2h_4-2h_5-46h_0-3h_6-3h_7 \end{pmatrix}$$
$$\approx \frac{2m}{\alpha}\begin{pmatrix} 6832 \text{ MeV} & -4434 \text{ MeV} \\ -4434 \text{ MeV} & 15979 \text{ MeV} \end{pmatrix}.$$

In contrast, the Moscow potential has very strong attraction and sustains, apart from the deuteron bound state, a very deep bound state known as the Pauli forbidden state (PFS). In this case expansion (54) begins from the second term,

$$\|b_{\ell\ell'}\| = 2m\begin{pmatrix} V_1+V_2\frac{\gamma}{\beta} & 6\sqrt{2}V_2\frac{\gamma^3}{\beta^3} \\ 6\sqrt{2}V_2\frac{\gamma^3}{\beta^3} & V_1+V_2\frac{\gamma}{\beta}(1-6\frac{\gamma^2}{\beta^2}) \end{pmatrix} \approx 2m\begin{pmatrix} -513 \text{ MeV} & -7156 \text{ MeV} \\ -7156 \text{ MeV} & 4547 \text{ MeV} \end{pmatrix}.$$

Both potentials describe the deuteron properties and the np-scattering quite well despite their completely different short-range behaviour.

First we considered real energies corresponding to bound and scattering states. We integrated equations (35) by the Runge–Kutta method from $r_{\min} = 10^{-4}$ fm to $r_{\text{int}} = 1$ fm with the boundary conditions $\|A^{(4)}(k, r_{\min})\|$ and $\|B^{(4)}(k, r_{\min})\|$. Then from $r_{\text{int}} = 1$ fm we integrated equations (17) up to $r_{\max} = 20$ 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

$$\det \|F^{(-)}(k, r_{\max})\| = 0 \tag{59}$$

is fulfilled at the points k_0 given in table 1. The binding energies and the percentages of the D-waves (D%) are also given in this table. For comparison table 1 contains the energies and D% obtained originally in [16–18] by the authors that constructed these potentials. Other observables such as the mean square radius and the electric quadrupole moment of the deuteron are also the same as those given in [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 wavefunction has a node at $r_c \sim 0.59$ fm.

For real positive k, i.e. for scattering states, we performed calculations with the same $r_{\min}$, r_{int}, and $r_{\max}$. According to equation (46) the product

$$\|F^{(+)}(k, r_{\max})\| \cdot \|F^{(-)}(k, r_{\max})\|^{-1} = \|S(k)\|$$

gives us the S-matrix which contains information about the scattering observables. The NN S-matrix is usually parametrized in terms of the so-called *bar* phase shifts and mixing parameter, introduced in [19], as follows

$$\begin{pmatrix} S_{00} & S_{02} \\ S_{20} & S_{22} \end{pmatrix} = \begin{pmatrix} e^{2i\bar{\delta}_0}\cos 2\bar{\varepsilon} & ie^{i(\bar{\delta}_0+\bar{\delta}_2)}\sin 2\bar{\varepsilon} \\ ie^{i(\bar{\delta}_0+\bar{\delta}_2)}\sin 2\bar{\varepsilon} & e^{2i\bar{\delta}_2}\cos 2\bar{\varepsilon} \end{pmatrix}.$$

From this matrix equation one obtains

$$\bar{\delta}_0 = \frac{\ln S_{00}}{2i}\sqrt{1-\frac{S_{02}^2}{S_{00}S_{22}}}$$

$$\bar{\delta}_2 = \frac{\ln S_{22}}{2i}\sqrt{1-\frac{S_{02}^2}{S_{00}S_{22}}}$$

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

The obtained phase shifts and mixing parameters are in agreement with the values given in [16], for all collision energies examined (up to $E_{\text{c.m.}} = 176$ MeV). For example, at $E_{\text{c.m.}} = 12$ MeV ($k = 0.537\,93$ fm^{-1}) the RSC potential gives†

$$\|F^{(\pm)}(k, r_{\max})\| = \begin{pmatrix} 0.162\,47\times 10^{11} \mp i0.183\,86\times 10^{12} & -0.609\,05\times 10^{5} \pm i0.689\,23\times 10^{6} \\ -0.133\,90\times 10^{13} \pm i0.610\,83\times 10^{11} & 0.501\,94\times 10^{7} \mp i0.228\,98\times 10^{6} \end{pmatrix}$$

and

$$\|S(k)\| = \begin{pmatrix} -0.956\,40 + i0.285\,07 & -0.062\,32 + i0.012\,29 \\ -0.062\,32 + i0.012\,29 & 0.993\,03 - i0.099\,33 \end{pmatrix}.$$

From the latter S-matrix we obtain the following scattering parameters

$$\bar{\delta}_0 = 1.4288 \qquad \bar{\delta}_2 = -0.049\,95 \qquad 2\bar{\varepsilon} = 0.063\,57$$

which are practically the same as those obtained by Reid [16]

$$\bar{\delta}_0 = 1.426 \qquad \bar{\delta}_2 = -0.050 \qquad 2\bar{\varepsilon} = 0.064$$

via a direct solution of the Schrödinger equation.

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

$$\|F^{(\pm)}(k, r_{\max})\| = \begin{pmatrix} -361.16 \pm i4347.4 & -0.084\,58 \pm i1.0183 \\ 30\,864 \mp i1423.1 & 7.2291 \mp i0.333\,31 \end{pmatrix}$$

but practically the same S-matrix

$$\|S(k)\| = \begin{pmatrix} -0.955\,57 + i0.287\,72 & -0.062\,83 + i0.012\,52 \\ -0.062\,83 + i0.012\,52 & 0.992\,68 - i0.100\,59 \end{pmatrix}$$

and therefore the same phase shifts and mixing parameter

$$\bar{\delta}_0 = 1.4275 \qquad \bar{\delta}_2 = -0.050\,59 \qquad 2\bar{\varepsilon} = 0.064\,11.$$

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 $F^{(\pm)}_{[\ell][\ell']}(k,r)$. To demonstrate an opposite example,

† The calculated $\|F^{(+)}(k, r_{\max})\|$ and $\|F^{(-)}(k, r_{\max})\|$ are complex conjugate to each other at least within five digits.

we solved equations (17) at the same energy ($E_{\text{c.m.}} = 12$ MeV) with a rudimentary NN potential (also in the deuteron channel) consisting of two Yukawa-type terms [20],

$$V(r) = v_c \frac{\exp(-\omega r/\rho_c)}{r/\rho_c} + v_t \frac{\exp(-\omega r/\rho_t)}{r/\rho_t} S_{12} \tag{60}$$

with

$$v_c = -22.7 \text{ MeV} \qquad v_t = -10.9 \text{ MeV}$$
$$\omega = 2.12 \qquad \rho_c = 2.47 \text{ fm} \qquad \rho_t = 3.68 \text{ fm}.$$

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 (54) are two orders of magnitude less than those for the RSC potential. As a result the Jost matrices calculated at $E_{\text{c.m.}} = 12$ MeV are

$$\|F^{(\pm)}(k, r_{\max})\| = \begin{pmatrix} 0.273\,28 \pm \text{i}0.878\,45 & 0.112\,04 \pm \text{i}0.237\,30 \\ 3.8437 \mp \text{i}0.376\,53 & 1.687\,6 \mp \text{i}0.156\,58 \end{pmatrix}$$

while the S-matrix is

$$\|S(k)\| = \begin{pmatrix} -0.987\,55 + \text{i}0.105\,46 & 0.115\,64 - \text{i}0.015\,980 \\ 0.115\,64 - \text{i}0.015\,980 & 0.979\,14 - \text{i}0.166\,31 \end{pmatrix}$$

are $\bar{\delta}_0 = 1.53$, $\bar{\delta}_2 = -0.0847$, and $\bar{\varepsilon}_0 = 0.117$.

Heretofore we have dealt with momenta on and above the real axis ($\text{Im}\, k \geqslant 0$) and therefore the coordinate rotation (29) was not needed. Consider now a point k which is under the real axis. To obtain the Jost matrix $\|\mathcal{F}^{(-)}(k)\|$ in this domain of the k-plane, we must integrate the rotated equations (30) (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 $\|F^{(\pm)}\|$ with their linear combinations (33) and the equations (30) with the corresponding linear combinations of them. The resulting rotated equations for $\|A\|$ and $\|B\|$ as well as the rotated iterative equations follow immediately from (35), (36), and (37) after simple replacement of r by $x\exp(\text{i}\theta)$.

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 $k = 0.5\exp(-\text{i}0.3\pi)$ fm^{-1}, i.e. at $E_{\text{c.m.}} \approx (-3.20 - \text{i}9.86)$ MeV, with three different values of the rotation angle: $\theta = 0, 0.35\pi, 0.4\pi$. The results obtained are given in table 2. The first line of this table demonstrates that the unrotated equations cannot give a correct θ-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, θ is large enough, such that $\text{Im}\, kr \geqslant 0$ and the point k is above the dividing line, then $\|F^{(-)}(k, x_{\max}\text{e}^{\text{i}\theta})\|$ does not depend on θ (compare the second and third lines of the table) and $x_{\max}$. To achieve the $x_{\max}$-independence when $\theta \neq 0$, we have to go further afield because the potential vanishes along the $x\exp(\text{i}\theta)$ slower than along the real r. Thus, the results given in table 2 were obtained with $x_{\max} = 50$ fm.

The number of digits which are unchanged under the rotation show the accuracy achieved. It is interesting to note in this connection that the accuracy of the second column of the Jost matrix as well as of the determinant always turn out to be much higher than that of the Jost matrix first column. This is exemplified in the last two lines of table 2. It is interesting to note 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 1) can be obtained even with boundary

Table 2. Jost matrix for the RSC potential at $k = 0.5\exp(-\mathrm{i}0.3\pi)$ fm^{-1}, calculated with $x_{\max} = 50$ fm and three different values of the rotation angle θ.

θ	$\|F^{(-)}(k, x_{\max}\mathrm{e}^{\mathrm{i}\theta})\|$
0	$\begin{pmatrix} 22\,637\,458\,292\,890 + \mathrm{i}14\,763\,693\,403\,731 & -22\,818\,484 + \mathrm{i}84\,501\,579 \\ 8\,536\,691\,059\,869 + \mathrm{i}6\,193\,286\,881\,927 & -10\,532\,586 + \mathrm{i}32\,492\,267 \end{pmatrix}$
0.35π	$\begin{pmatrix} -325\,291\,222\,087 + \mathrm{i}639\,117\,048\,997 & -2\,294\,097 - \mathrm{i}362\,305 \\ 145\,085\,673\,415 - \mathrm{i}1\,488\,370\,181\,212 & 4\,729\,536 - \mathrm{i}1\,042\,674 \end{pmatrix}$
0.40π	$\begin{pmatrix} -325\,288\,820\,471 + \mathrm{i}639\,116\,901\,481 & -2\,294\,097 - \mathrm{i}362\,305 \\ 145\,081\,315\,229 - \mathrm{i}1\,488\,368\,045\,635 & 4\,729\,536 - \mathrm{i}1\,042\,675 \end{pmatrix}$

conditions $\|A^{(1)}(k, r_{\min})\|$ and $\|B^{(1)}(k, r_{\min})\|$ when the first column of $\|F^{(-)}(k, r_{\max})\|$ is even wrong. The only explanation for this is that somehow both elements of this column find the same erroneous term which cancels 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 wavefunctions.

None of the potentials (57), (58), (60) generate resonances (at least at reasonably low energies). To the best of our knowledge, non-central potentials generating resonances have not yet been published. 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

$$V_c(r) = 7.5r^2\exp(-r) \tag{61}$$

which is widely used as a testing case for new methods that locate resonances (see for example [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 $\hbar^2/2m = \frac{1}{2}$ 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 [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

$$\|W_{\ell\ell'}(r)\| = 2m\begin{pmatrix} 7.5r^2\exp(-r) & -\lambda r^2\exp(-r) \\ -\lambda r^2\exp(-r) & -\lambda r^2\exp(-r) \end{pmatrix} \tag{62}$$

should generate resonances at least when λ is small. Bound states can also be generated by increasing λ since we have chosen a negative sign for the D-wave potential and for the off-diagonal elements of the matrix (62).

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 λ up to the value $\lambda = 15$ MeV. The resulting spectrum is given in table 3 and depicted in figure 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 figure 2 we also show the positions of the first three resonances when $\lambda = 0$ which coincide with the resonances of the potential (61) found in [7]. The small open circles show their movement when λ is gradually increased in steps of $\Delta\lambda = 1$ MeV. The digits displayed in table 3 are those which do not change when the rotation angle changes and thus they represent the accuracy of our calculations.

Table 3. Spectral points of the model potential (see text) with $\lambda = 15$ MeV.

Re p_0 (fm^{-1})	Im p_0 (fm^{-1})	E_0 (MeV)	Γ (MeV)
0	4.558 153 1714	−10.388 380 1672	0
0	4.023 079 863	−8.092 585 79	0
0	3.471 206 989	−6.024 638 98	0
0	2.899 849 780	−4.204 564 37	0
0	2.305 427 868	−2.657 498 83	0
0	1.681 898 798	−1.414 391 78	0
0	1.016 190 35	−0.516 321 4	0
0	0.254 097	−0.032 282 6	0
3.446 608 92	−0.530 114 39	5.799 045 90	3.654 194 0
4.138 807 8309	−0.146 714 8600	8.554 102 5053	1.214 449 223
4.465 210 96	−0.686 071 761	9.733 707 24	6.126 910 30
4.744 324	−1.332 365	10.366 71	12.642 34
4.963 56	−1.997 19	10.324 1	19.826 3
5.141 0	−2.663 4	9.668 1	27.385

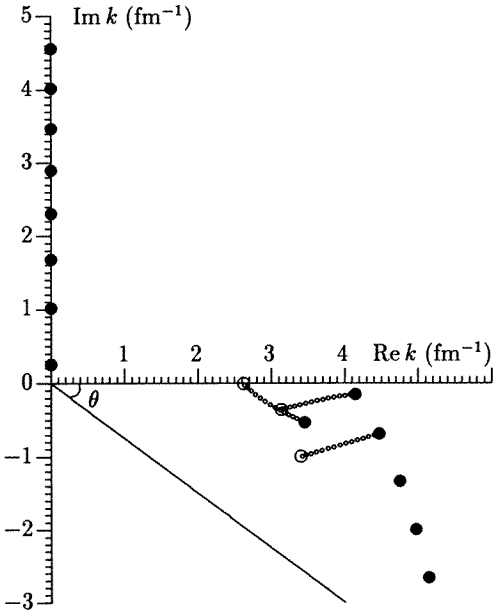

Figure 2. Spectral points (full circles) of the model potential with $\lambda = 15$ MeV. The large open circles represent three of the resonances generated by the central potential V_c and the small open circles show the movement of the resonances when λ decreases from 15 to 0 MeV in steps of $\Delta\lambda = 1$ MeV. The dividing line corresponds to $\theta = 0.2\pi$.

5. Conclusions

This 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. We have extended it here 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 reveals new possibilities in locating resonances. Within this method the Siegert wavefunctions can be properly normalized. Even subthreshold 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 ℓ and therefore Regge trajectories can also be located [7].

The wavefunction 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 [6, 7]. To do this we need only replace, in all formulae, the Riccati–Bessel functions with the corresponding Coulomb functions.

The method can be extended further: first, to treat the N-body coupled hyper-radial equations which differ from the two-body radial equations only by the possibility of having half-integer values of ℓ; 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 extentions is under way.

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Appendix. 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 equation (11),

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

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

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

A.1. Behaviour at short distances

The property (ii) implies that the boundary condition (12) should be imposed at the point $r=0$. Equation (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 $r \geqslant \delta > 0$ for any arbitrary small δ. 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), equations (11) decouple giving

$$[r^2\partial_r^2 - \ell(\ell+1)]\Phi_{[\ell][\ell']}(k,r) \approx 0 \qquad r\in[0,\delta]. \tag{A1}$$

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 equation (A1) with linearly independent columns, is to choose its diagonal as follows

$$\|\Phi(k,r)\| \underset{r\to 0}{\sim} \begin{pmatrix} r^{\ell_1+1} & 0 & \cdots & 0 \\ 0 & r^{\ell_2+1} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & r^{\ell_N+1} \end{pmatrix} \tag{A2}$$

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

$$\begin{pmatrix} \Phi_{[\ell_1][\ell_n]}(k,r) \\ \Phi_{[\ell_2][\ell_n]}(k,r) \\ \vdots \\ \Phi_{[\ell_n][\ell_n]}(k,r) \\ \vdots \\ \Phi_{[\ell_N][\ell_n]}(k,r) \end{pmatrix} \underset{r\to 0}{\sim} \begin{pmatrix} 0 \\ 0 \\ \vdots \\ r^{\ell_n+1} \\ \vdots \\ 0 \end{pmatrix}. \tag{A3}$$

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

$$\|\Phi(k,r)\| \underset{r\to 0}{\sim} \begin{pmatrix} r^{\ell_1+1} & \mathrm{o}(r^{\ell_2+1}) & \cdots & \mathrm{o}(r^{\ell_N+1}) \\ \mathrm{o}(r^{\ell_1+1}) & r^{\ell_2+1} & \cdots & \mathrm{o}(r^{\ell_N+1}) \\ \vdots & \vdots & \vdots & \vdots \\ \mathrm{o}(r^{\ell_1+1}) & \mathrm{o}(r^{\ell_2+1}) & \cdots & r^{\ell_N+1} \end{pmatrix}. \tag{A4}$$

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

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

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

$$\det\|\Phi(k,r)\| \underset{r\to 0}{\longrightarrow} \prod_i r^{\ell_i+1}$$

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

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

$$\lim_{r\to 0} \frac{\Phi_{[\ell][\ell']}(k,r)}{r^{\ell'+1}} = \delta_{[\ell][\ell']}. \tag{A5}$$

Since we can choose the normalization 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 find the boundary condition in the form

$$\lim_{r\to 0}\frac{\Phi_{[\ell][\ell']}(k,r)}{j_{\ell'}(kr)}=\delta_{[\ell][\ell']}. \tag{A6}$$

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

$$h_\ell^{(+)}(kr)F^{(+)}_{[\ell][\ell']}(k,r)\underset{r\to 0}{\longrightarrow}-h_\ell^{(-)}(kr)F^{(-)}_{[\ell][\ell']}(k,r)$$

and the Lagrange condition (16) gives

$$h_\ell^{(+)}(kr)\partial_r F^{(+)}_{[\ell][\ell']}(k,r)=-h_\ell^{(-)}(kr)\partial_r F^{(-)}_{[\ell][\ell']}(k,r).$$

On the other hand

$$\frac{h_\ell^{(+)}(kr)}{h_\ell^{(-)}(kr)}\equiv\frac{j_\ell(kr)+\mathrm{i}n_\ell(kr)}{j_\ell(kr)-\mathrm{i}n_\ell(kr)}\underset{r\to 0}{\longrightarrow}-1$$

from which we conclude that for $r\sim 0$ the matrices $\|F^{(+)}(k,r)\|$ and $\|F^{(-)}(k,r)\|$ and their first derivatives become identical, i.e.

$$\|F^{(+)}(k,r)\|\underset{r\to 0}{\longrightarrow}\|F^{(-)}(k,r)\| \tag{A7}$$

$$\partial_r\|F^{(+)}(k,r)\|\underset{r\to 0}{\longrightarrow}\partial_r\|F^{(-)}(k,r)\|. \tag{A8}$$

The convergence rate is different for different matrix elements (see the proof at the end of this section). However, for all of them, due to (A8), at least the leading terms of the series expansions of $\|F^{(+)}(k,r)\|$ and $\|F^{(-)}(k,r)\|$ must coincide. Explicitly we have

$$\Phi_{[\ell][\ell']}(k,r)\underset{r\to 0}{\longrightarrow}\tfrac{1}{2}[h_\ell^{(+)}(kr)+h_\ell^{(-)}(kr)]A_{[\ell][\ell']}(k,r)=j_\ell(kr)A_{[\ell][\ell']}(k,r) \tag{A9}$$

where the matrix $\|A(k,r)\|$ describes the (common) short-range behaviour of $\|F^{(\pm)}(k,r)\|$.

Comparing equations (A7) and (A9) with equation (A6), we find the following boundary conditions for the matrices $\|F^{(\pm)}(k,r)\|$

$$\lim_{r\to 0}\frac{j_\ell(kr)F^{(\pm)}_{[\ell][\ell']}(k,r)}{j_{\ell'}(kr)}=\delta_{[\ell][\ell']}. \tag{A10}$$

Note that unlike (A6), these conditions do not demand that all of the elements of the matrices $\|F^{(\pm)}\|$ be regular. Indeed, when $\ell>\ell'$ equation (A10) holds even if $F^{(\pm)}_{[\ell][\ell']}(k,r)\sim r^{-(\ell-\ell'-\epsilon)}$ 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, equation (15), the functions $F^{(\pm)}_{[\ell][\ell']}(k,r)$ are closely related to the Jost solutions and thus their singular behaviour is not surprising. The $\Phi_{[\ell][\ell']}(k,r)$ itself always remains regular due to the presence of $j_\ell(kr)$ in (A9) which compensates for the diverging terms.

Equation (A10) 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 $F^{(\pm)}_{[\ell][\ell']}\sim \mathrm{o}(j_\ell/j_{\ell'})$. To obtain them explicitly, let us take indefinite integrals in both sides of equations (17). This gives

$$F^{(\pm)}_{[\ell][\ell']}(k,r)=\text{constant}\pm\frac{1}{\mathrm{i}k}\int h_\ell^{(\mp)}(kr)\sum_{[\ell'']}W_{[\ell][\ell'']}(r)\Phi_{[\ell''][\ell']}(k,r)\,\mathrm{d}r. \tag{A11}$$

The integration constants are fixed for the diagonal and the right-top corner elements by the conditions (A10). Indeed, due to (5) the integrals in (A11) for $\ell \leqslant \ell'$ give functions ($\int r^{-\ell} r^{-2+\varepsilon} r^{\ell'+1}\,\mathrm{d}r$, $\varepsilon > 0$) which vanish at $r = 0$. Hence to fulfil (A10) we must set constant $= 1$ for $\ell = \ell'$ and constant $= 0$ for $\ell < \ell'$. For the left-bottom elements we still have to choose the normalization which is fixed by letting constant $= \delta_{[\ell][\ell']}$. Thus finally

$$F^{(\pm)}_{[\ell][\ell']}(k,r) = \delta_{[\ell][\ell']} \pm \frac{1}{\mathrm{i}k} \int h^{(\mp)}_{\ell}(kr) \sum_{[\ell'']} W_{[\ell][\ell'']}(r)\Phi_{[\ell''][\ell']}(k,r)\,\mathrm{d}r \qquad \text{(A12)}$$

where the indefinite integrals should be understood as primitive functions since all arbitrary constants have already been fixed.

Consider now equations (A12) 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 $W_{[\ell][\ell']}(r)$, for $\Phi_{[\ell][\ell']}(k,r)$ only the diagonal elements are known,

$$\Phi_{[\ell][\ell]}(k,r) \approx j_{\ell}(kr) \qquad r \in (0,\delta].$$

Equation (A4) shows that the elements of the matrix $\|\Phi\|$ vanish (when $r \to 0$) with different speeds. In particular, this speed increases from left to right in each row. 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 for the diagonal element. Looking at either the differential equations (17) or the integral equations (A12), we note 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

$$\Phi^{(0)}_{[\ell][\ell']}(k,r) = j_{\ell}(kr)\delta_{[\ell][\ell']} \qquad r \in [0,\delta] \qquad \text{(A13)}$$

which, according to (A9), implies that

$$F^{(\pm)(0)}_{[\ell][\ell']}(k,r) = \delta_{[\ell][\ell']} \qquad r \in [0,\delta]. \qquad \text{(A14)}$$

Substituting (A13) into the indefinite integral (A12) and using the series expansions of h_{ℓ}, j_{ℓ}, and $W_{[\ell][\ell']}$, we obtain the first iteration $\|F^{(\pm)(1)}\|$ for all elements of the matrices $\|F^{(\pm)}\|$ and thus we find $\|\Phi^{(1)}\|$ 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 use of the following recurrence formulae

$$F^{(\pm)(n+1)}_{[\ell][\ell']}(k,r) = \delta_{[\ell][\ell']} \pm \frac{1}{\mathrm{i}k} \int h^{(\mp)}_{\ell}(kr) \sum_{[\ell'']} W_{[\ell][\ell'']}(r)\Phi^{(n)}_{[\ell''][\ell']}(k,r)\,\mathrm{d}r \qquad \text{(A15)}$$

$$\Phi^{(n)}_{[\ell][\ell']}(k,r) = \tfrac{1}{2}[h^{(+)}_{\ell}(kr)F^{(+)(n)}_{[\ell][\ell']}(k,r) + h^{(-)}_{\ell}(kr)F^{(-)(n)}_{[\ell][\ell']}(k,r)]. \qquad \text{(A16)}$$

Now we can show how fast the matrices $\|F^{(+)}(k,r)\|$ and $\|F^{(-)}(k,r)\|$ converge to each other when $r \to 0$. According to equation (33) we have

$$\|F^{(\pm)}(k,r)\| \equiv \|A(k,r)\| \pm \mathrm{i}\|B(k,r)\|.$$

The series expansions of the matrices $\|A\|$ and $\|B\|$ at short distances can be obtained iteratively using equations (36) and (37) which are equivalent to equations (A14)–(A16). The leading terms of these expansions are defined by the indefinite integrals (primitive functions)

$$A^{(1)}_{[\ell][\ell']}(k,r) = \delta_{[\ell][\ell']} - \frac{1}{k}\int n_{\ell}(kr)W_{[\ell][\ell']}(r)\,j_{\ell'}(kr)\,\mathrm{d}r$$

$$B^{(1)}_{[\ell][\ell']}(k,r) = -\frac{1}{k}\int j_{\ell}(kr)W_{[\ell][\ell']}(r)\,j_{\ell'}(kr)\,\mathrm{d}r$$

where the functions $j_\ell(kr)$, $n_\ell(kr)$ and $W_{[\ell][\ell']}(r)$ should be replaced by their series expansions. The above equations can be rewritten as

$$A^{(1)}_{[\ell][\ell']}(k,r) = \delta_{[\ell][\ell']} + \mathcal{O}\left(\int W_{[\ell][\ell']}(r) r^{\ell'-\ell+1}\, \mathrm{d}r \right)$$

$$B^{(1)}_{[\ell][\ell']}(k,r) = \mathcal{O}\left(\int W_{[\ell][\ell']}(r) r^{\ell'+\ell+2}\, \mathrm{d}r \right).$$

Taking into account the condition (5), we get that the matrix

$$B_{[\ell][\ell']}(k,r) = \mathcal{O}\left(\int r^{\ell'+\ell+\varepsilon}\, \mathrm{d}r \right) \qquad \varepsilon > 0$$

where ε defines the short-range behaviour of the potential $W(r) \sim r^{\varepsilon-2}$, always vanishes at short distances and that

$$B_{[\ell][\ell']}(k,r) = \mathrm{o}(A_{[\ell][\ell']}(k,r)) \qquad \forall\ [\ell], [\ell'].$$

For the diagonal matrix elements the greater the ε is, the faster the second term of $\|F^{(\pm)}\| \equiv \|A\| \pm \mathrm{i}\|B\|$ vanishes. The rate at which the off-diagonal elements vanish depends only on the column number, i.e.

$$\frac{B_{[\ell][\ell']}(k,r)}{A_{[\ell][\ell']}(k,r)} = \mathcal{O}\left(\frac{r^{\ell'+\ell+\varepsilon+1}}{\delta_{[\ell][\ell']} + r^{\ell'-\ell+\varepsilon}} \right) = \begin{cases} \mathcal{O}(r^{2\ell+1+\varepsilon}) & [\ell'] = [\ell] \\ \mathcal{O}(r^{2\ell+1}) & [\ell'] \neq [\ell]. \end{cases} \tag{A17}$$

In section 4 we give the series expansions for the matrices $\|A\|$, $\|B\|$, and $\|\Phi\|$ explicitly for a potential which couples two partial waves and for $\varepsilon = 1$.

A.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

$$\partial_r F^{(\pm)}_{[\ell][\ell']}(k,r) = \pm \frac{1}{\mathrm{i}k} h^{(\mp)}_\ell(kr) \sum_{[\ell'']} W_{[\ell][\ell'']}(r) \Phi_{[\ell''][\ell']}(k,r). \tag{A18}$$

Since the right-hand sides of these equations involve the basic solutions $\Phi_{[\ell][\ell']}(k,r)$, we need to know how these solutions behave in different domains of the k-plane when $r \to \infty$. To this end we consider equation (11) at large r. If the potential is of short range (decaying exponentially or faster) these equations are reduced to the uncoupled Riccati–Bessel equations, namely,

$$[\partial_r^2 + k^2 - \ell(\ell+1)/r^2]\Phi_{[\ell][\ell']}(k,r) \underset{r\to\infty}{\longrightarrow} 0. \tag{A19}$$

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

$$\|h^{(\pm)}(kr)\| \equiv \begin{pmatrix} h^{(\pm)}_{\ell_1}(kr) & 0 & \cdots & 0 \\ 0 & h^{(\pm)}_{\ell_2}(kr) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & h^{(\pm)}_{\ell_N}(kr) \end{pmatrix}. \tag{A20}$$

Any other solution is a linear combination of them. Therefore

$$\|\Phi(k,r)\| \underset{r\to\infty}{\longrightarrow} \|h^{(+)}(kr)\| \cdot \|C_+\| + \|h^{(-)}(kr)\| \cdot \|C_-\| \tag{A21}$$

and according to (26)

$$\|\Phi(k,r)\| \underset{r\to\infty}{\longrightarrow} \exp(\mathrm{i}kr)\|\tilde{C}_+\| + \exp(-\mathrm{i}kr)\|\tilde{C}_-\|. \tag{A22}$$

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

$$|\Phi_{[\ell][\ell']}(k,r)| \leqslant \text{constant} \qquad \forall \ell, \ell' \qquad \text{when } r \to \infty. \tag{A23}$$

For $\operatorname{Im} kr \neq 0$, the regular solution diverges due either to the first or the second term of (A22). In this case we can keep only the diverging term of it, namely,

$$\|\Phi(k,r)\| \underset{r\to\infty}{\sim} \exp(-\mathrm{i}kr)\|\tilde{C}_-\| \qquad \operatorname{Im} kr > 0 \tag{A24}$$

$$\|\Phi(k,r)\| \underset{r\to\infty}{\sim} \exp(+\mathrm{i}kr)\|\tilde{C}_+\| \qquad \operatorname{Im} kr < 0. \tag{A25}$$

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 (A21), i.e.

$$\|\Phi(k_0,r)\| \underset{r\to\infty}{\overset{\text{def}}{\longrightarrow}} \exp(+\mathrm{i}k_0 r)\|\tilde{C}_+\|. \tag{A26}$$

Spectral points situated on the positive imaginary axis correspond to bound states, and those situated under the real axis to resonance states.

Although we have derived equations (A23)–(A25) 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.

Using equations (A22), (A24)–(A26), and the asymptotic form of the Riccati–Hankel functions, equation (26), together with the constraint on the long-range behaviour of the potential, $W(r) \propto r^{-(1+\epsilon)}$, $\epsilon > 0$, we find from equation (A18) that in general the derivatives of $\|F^{(+)}(k,r)\|$ and $\|F^{(-)}(k,r)\|$ vanish or grow exponentially in the different domains of the k-plane, namely

$$\partial_r \|F^{(+)}(k,r)\| \underset{r\to\infty}{\propto} \begin{cases} \dfrac{\exp(-2\mathrm{i}kr)}{r^{1+\epsilon}} & \operatorname{Im} kr > 0 \\ \dfrac{\|\tilde{C}_+\| + \exp(-2\mathrm{i}kr)\|\tilde{C}_-\|}{r^{1+\epsilon}} & \operatorname{Im} kr = 0 \\ \dfrac{1}{r^{1+\epsilon}} & \operatorname{Im} kr < 0 \end{cases} \tag{A27}$$

$$\partial_r \|F^{(-)}(k,r)\| \underset{r\to\infty}{\propto} \begin{cases} \dfrac{1}{r^{1+\epsilon}} & \operatorname{Im} kr > 0 \\ \dfrac{\exp(2\mathrm{i}kr)\|\tilde{C}_+\| + \|\tilde{C}_-\|}{r^{1+\epsilon}} & \operatorname{Im} kr = 0 \\ \dfrac{\exp(2\mathrm{i}kr)}{r^{1+\epsilon}} & \operatorname{Im} kr < 0. \end{cases} \tag{A28}$$

It is clear that $\|F^{(+)}(k,r)\|$ and $\|F^{(-)}(k,r)\|$ have no limits at $r = \infty$ when $\operatorname{Im} kr > 0$ and $\operatorname{Im} kr < 0$ respectively because their derivatives grow exponentially in these domains. In the mirror domains, $\operatorname{Im} kr < 0$ and $\operatorname{Im} kr > 0$, these derivatives vanish rapidly enough to guarantee the existence of limits. Indeed, the behaviour

$$\frac{\mathrm{d}\varphi(r)}{\mathrm{d}r} \underset{r\to\infty}{\sim} r^{-(\epsilon+1)} \qquad \epsilon > 0$$

of the derivative of a function $\varphi(r)$ is a sufficient condition for the existence of its limit at large r since the asymptotic behaviour of the function itself can be written as

$$\varphi(r) \underset{r\to\infty}{\sim} \int r^{-(\epsilon+1)}\,\mathrm{d}r = \left(\text{constant} - \frac{1}{\epsilon r^{\epsilon}}\right) \underset{r\to\infty}{\longrightarrow} \text{constant}.$$

On the dividing line, $\operatorname{Im} kr = 0$, which separates the mirror domains, both derivatives

$$\partial_r \|F^{(\pm)}(k,r)\| \underset{r\to\infty}{\propto} \frac{\exp(\mp 2\mathrm{i}kr)\|\tilde{C}_{\mp}\| + \|\tilde{C}_{\pm}\|}{r^{1+\epsilon}} \tag{A29}$$

oscillate with vanishing amplitude. From the above equation it follows that

$$\|F^{(\pm)}(k,r)\| = \|F^{(\pm)}(k,R)\| + \text{constant}\int_R^r \frac{\exp(\mp 2\mathrm{i}k\rho)\|\tilde{C}_{\mp}\| + \|\tilde{C}_{\pm}\|}{\rho^{1+\epsilon}}\,\mathrm{d}\rho \tag{A30}$$

where R is a sufficiently large radius beyond which the asymptotic behaviour (A29) is valid. Therefore on the dividing line the limits $\|F^{(\pm)}(k,\infty)\|$ exist, because the integral in equation (A30) converges. The last is obvious since

$$\int_R^r \left|\frac{\exp(\mp 2\mathrm{i}k\rho)}{\rho^{1+\epsilon}}\right| \mathrm{d}\rho = \frac{1}{\epsilon R^{\epsilon}} - \frac{1}{\epsilon r^{\epsilon}}.$$

At spectral points we have

$$\partial_r \|F^{(+)}(k,r)\| \underset{r\to\infty}{\propto} \frac{1}{r^{1+\epsilon}} \qquad \partial_r \|F^{(-)}(k,r)\| \underset{r\to\infty}{\propto} \frac{\exp(2\mathrm{i}k_0 r)}{r^{1+\epsilon}}$$

which implies that $\|F^{(+)}(k,r)\|$ has a limit at all of them. In contrast $\|F^{(-)}(k,r)\|$ has a limit only at those points situated above or on the dividing line. Therefore the only points where both limits $\lim_{r\to\infty}\|F^{(\pm)}(k,r)\|$ exist simultaneously are those with $\operatorname{Im} kr = 0$ and the spectral points with $\operatorname{Im} kr > 0$.

For real r then $\lim_{r\to\infty}\|F^{(+)}(k,r)\|$ exists for $\operatorname{Im} k \leqslant 0$ and at the spectral points, while $\lim_{r\to\infty}\|F^{(-)}(k,r)\|$ exists for $\operatorname{Im} k \geqslant 0$. In this case the dividing line that separates the two domains of the k-plane coincide with the real axis. This line can be turned downwards, to expose the resonance spectral points, by rotating r as given by equation (29). Indeed, if ϕ is the polar angle parametrizing a point on the k-plane

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

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

$$\operatorname{Im} kr = \operatorname{Im}(|k|x\mathrm{e}^{\mathrm{i}(\phi+\theta)}) = |k|x\sin(\theta+\phi) \tag{A31}$$

positive even when ϕ is negative, $-\theta \leqslant \phi \leqslant \pi - \theta$, 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 $[-\infty\mathrm{e}^{-\mathrm{i}\theta}, +\infty\mathrm{e}^{-\mathrm{i}\theta}]$ (see figure 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 $\lim_{r\to\infty}\|F^{(+)}(k,r)\|$ 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 (A18) behaves, below the dividing line ($\operatorname{Im} kr < 0$), as

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

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

$$|k| \sin(\theta + \phi) > -\frac{\mu}{2} \cos\theta. \tag{A32}$$

If $\theta = 0$, this condition reads $\mathrm{Im}\, k > -\mu/2$ which enables us to also locate virtual states (spectral points on the negative imaginary axis) situated not far from the origin.

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