Finite-rank potential that reproduces the Padé approximant

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If a scattering potential is of a finite rank, say N, the exact solution of the problem can be obtained from the Born series, if the potential strength is within the radius of convergence; the exact solution can be obtained from the analytical continuation of the formal Born series outside the radius of convergence. Beyond the first $2N$ terms of the Born series, an individual term of the Born series depends on the first $2N$ terms, and the $[N/N]$ Padé approximant and the exact solution agree with each other. The above-mentioned features of a finite-rank problem are relevant to scattering theory in general, because most scattering problems may be handled as an extension of the rank-N problem, in which the rank N tends to infinity. The foregoing aspects of scattering theory will be studied in depth in the present paper, and in so doing we proceed in the opposite direction. Namely, given a potential, we calculate the first $2N$ terms of the Born series for the K matrix and the first N terms of the Born series for the wave function. Using these data, a special rank-N potential is constructed in such a way that it reproduces the $[N/N]$ Padé approximant of the K matrix of the original scattering problem. One great advantage of obtaining such a rank-N potential is that the wave function of the system may be approximated in the same spirit as done for the K matrix; hence, we can introduce a new approximation method for dealing with an off-shell T matrix. A part of the mathematical work is incomplete, but the physical aspects are thoroughly discussed.

I. INTRODUCTION

The method of Padé approximants has been extensively used in recent years in scattering theory in various forms, e.g., in combination with the variational method.[1] Also, serious studies have been made to prove that the Padé approximant converges to the exact result as its rank tends to infinity, wherein the analytic property of the exact result as a function of the variable used in expansions is crucial.[2] We may accept, under certain conditions, that an interaction potential may be approximated by a potential of finite rank, such that the result based on the finite-rank approximation converges to the exact result in the limit as the rank tends to infinity.[3] Let us denote the potential strength by λ. We assume that the interaction is spherically symmetric so that each partial wave may be treated separately. Accepting the statements discussed in Ref. 3, we may assert that the partial-wave T matrix is a meromorphic function of λ, having only simple poles. Consequently the partial-wave K matrix may be set in the form

$$K(E)=\lambda\sum_{n=1}^{\infty}\lambda_n S_n/(\lambda_n-\lambda)=\lambda\sum_{n=1}^{\infty}S_n/(1-\lambda\eta_n)\,, \quad (1.1)$$

where

$$\eta_n=\lambda_n^{-1}\,. \quad (1.2)$$

The above equation shows that, when considered as a function of λ, the partial-wave K matrix has a simple pole at $\lambda=\lambda_n$. Both the position of the pole $\lambda_n=\lambda_n(E,l)$ and the residue parameter $S_n=S_n(E,l)$ are a function of energy E and angular momentum l of the partial wave. As will be discussed in Sec. II, η_n is an eigenvalue of the rescattering operator [cf. (2.22) and (2.26)], and S_n is obtained from the on-shell representation of the corresponding eigenfunction [(2.39)]. The integer n that labels an individual term is the radial quantum number. It counts the number of extra nodes of the wave function that are added to (or removed from) the wave function of a free particle by the attractive (repulsive) potential of strength λ_n.[4]

Let us consider the formal Born expansion of the K matrix

$$K(E)=(2/\pi)\sum_{n=1}^{\infty}\lambda^n K_n\,. \quad (1.3)$$

It is implied by Eq. (1.1) that the coefficient K_n in the Born series may be expressed in terms of η_n and S_n of (1.1). Hence, we have

$$(2/\pi)K_n=\sum_{m=1}^{\infty}S_m\eta_m{}^{n-1}=\sum_{m=1}^{\infty}S_m\lambda_m{}^{1-n}\,. \quad (1.4)$$

Suppose that the parameters λ_n of (1.1) may be ordered according to their magnitude so that

$$|\lambda_1|<|\lambda_2|<|\lambda_3|<\cdots\,, \quad (1.5)$$

and that the magnitude of λ_1 is the smallest. Using the right-hand-side (RHS) member of Eq. (1.4), one can readily show that the Born series (1.3) converges within the radius of convergence defined by

$$|\lambda| < |\lambda_1| . \tag{1.6}$$

Let us denote by $K^{[N/N]}$ the $[N/N]$ Padé approximant of the formal Born series, (1.3),

$$K^{[N/N]} = P_N/Q_N , \tag{1.7}$$

where both the numerator P_N and denominator Q_N are certain polynomials of λ of order N. Let us expand the RHS of (1.7) into a formal Born series

$$K^{[N/N]} = (2/\pi)\sum_{n=1}^{\infty} \lambda^n K_n^{[N/N]} . \tag{1.8}$$

The coefficients $K_n^{[N/N]}$ on the RHS of (1.8) are equal to the corresponding ones on the RHS of (1.3) from $n=1$ through $n=2N$

$$K_n^{[N/N]} = K_n, \quad 1 \leq n \leq 2N . \tag{1.9}$$

Both P_N and Q_N of (1.7) may be uniquely determined based on the conditions of (1.9).[5] If the first few zeros of the denominator Q_N are located in a close neighborhood of the corresponding first few λ_n's of (1.1), the analytic property as a function of λ of the Padé approximant $K^{[N/N]}$ may become close to that of the exact K matrix $K(E)$ of (1.1) in a certain domain of λ that includes λ_1 in its inside. Then, with a suitably large N, the $[N/N]$ Padé approximant may serve as a good approximation to the K matrix outside the convergence radius of the Born series

$$|\lambda| > |\lambda_1| . \tag{1.6a}$$

Therefore, assuming that the series of (1.1) converges rapidly, we truncate the series after the first N terms, denoting the truncated K matrix by $\tilde{K}_N$. Then, we should have

$$K \simeq \tilde{K}_N , \tag{1.10}$$

and furthermore, the form of $\tilde{K}_N$ as a function of λ is similar to the $[N/N]$ Padé approximant $K^{[N/N]}$ of (1.7),

$$\tilde{K}_N = \tilde{N}_N/\tilde{D}_N ; \tag{1.11}$$

the denominator $\tilde{D}_N$ has properties similar to those of Q_N of (1.7) and is given by

$$\tilde{D}_N = \prod_{n=1}^{N} (1 - \lambda\eta_n) . \tag{1.12}$$

To obtain several results that are comparable to the above, (1.10)–(1.12), let us consider a potential of rank N

$$(r|\, V'^{[N]} \,|r') = \lambda \sum_{n=1}^{N} f_n(r) f_n^{\dagger}(r') , \tag{1.13}$$

where $f_n(r)$, $n=1,\ldots,N$, are the form factors that define the separable potentials. Let the K matrix for the rank-N potential $\underline{V}'^{[N]}$, (1.13), be $K'^{[N]}$. The $K'^{[N]}$ takes a form of the same type as the N-term truncation of (1.1), i.e., $\tilde{K}_N$ of (1.11),

$$K'^{[N]} = \lambda \sum_{n=1}^{N} S_n'/(1 - \lambda\eta_n') , \tag{1.14}$$

where η_n' and S_n' are the pole and residue parameters, respectively, for the rank-N potential $\underline{V}'^{[N]}$. Let the $[N/N]$ Padé approximant for the $K'^{[N]}$ be presented in the form of P_N'/Q_N', in a fashion similar to the RHS of (1.7). Since the rank N is finite, the $[N/N]$ Padé approximant agrees with $K'^{[N]}$, the exact K matrix for $\underline{V}'^{[N]}$,

$$K'^{[N]} = P_N'/Q_N' , \tag{1.15}$$

where the denominator Q_N' is given by

$$Q_N' = \prod_{n=1}^{N} (1 - \lambda\eta_n') . \tag{1.16}$$

Furthermore, we may be able to choose a suitable set of form factors $f_n(r)$, $n=1,\ldots,N$, in (1.13), such that the parameters used in (1.14) become close to the corresponding quantities used in (1.1), or equivalently in (1.11),

$$\eta_n' \simeq \eta_n \text{ and } S_n' \simeq S_n, \quad 1 \leq n \leq N . \tag{1.17}$$

If these conditions are satisfied, the rank-N potential $\underline{V}'^{[N]}$, (1.13), may be substituted for the original potential $\underline{V}$ as its close approximation, a sufficient procedure as far as a partial wave at a fixed energy is concerned.

We have given a quick survey of three related subjects: (i) the Mittag-Leffler expansion of the partial-wave K matrix, (1.1), in which we consider the K matrix as a function of potential strength λ; (ii) the $[N/N]$ Padé approximant with a suitably large N, sketched with the help of (1.7)–(1.9); (iii) the rank-N approximation $\underline{V}'^{[N/N]}$ to be substituted for the original potential $\underline{V}$, briefly explained by (1.13)–(1.17). Our purpose is to bring these three aspects of scattering theory to an even stronger tie with each other, so to speak, so that we may establish a unified and transparent view of scattering theory as well as develop a powerful method of approximation. When the RHS's of (1.1), (1.7), and (1.14) are compared with each other, after a suitably large rank N and an adequate set of form factors $\{f_n(r)\}$ in (1.13) are chosen so that the conditions of (1.17) will be satisfied, we may be able to show

$$K(E) \approx K^{[N/N]} \approx K'^{[N]} . \tag{1.18}$$

Our major result is that, once the interaction potential $\underline{V}$ is given, one may obtain a special rank-N potential

$$\lambda(r|\,\Pi^{[N/N]}\,|r') = \lambda \sum_{n=1}^{N} \xi_n(r)\, \xi_n^{\dagger}(r') , \tag{1.19}$$

which automatically reproduces the $[N/N]$ Padé approximant $K^{[N/N]}$ of Eqs. (1.7)–(1.9). When limited to local potentials, the same result has been independently derived by Garibotti and Villani, whose starting point was to symmetrize the kernel of the Lippmann-Schwinger equation by using the square root of the absolute value of the potential.[6]

In this paper, we emphasize the usefulness of separable potentials,[7] and tackle our problem straightforwardly by using algebraic methods. In Sec. II, we review the method of the finite-rank-potential approximation, and discuss the foundation that enables us to obtain the results shown in (1.18). This review suggests how to choose the form-factor set $\{\xi_n(r)\}$ in (1.19). The square root of the interaction potential is completely avoided, and hence our results may be extended to relativistic scattering problems or to few-body problems. For convenience in application, all essential results will be written out explicitly, rather than giving them in the form of recurrence formulas.

II. THE HOMOGENEOUS LIPPMANN-SCHWINGER EQUATION AND EIGENFUNCTIONS USEFUL IN THE T-MATRIX THEORY

Our task is to analyze the algebraic relations that exist among functional-space elements obtained by iterating a kernel of scattering-theory integral equations. Even though we will limit ourselves to nonrelativistic scattering in the present paper, this will not harm the generality of our results. As long as a kernel may be iterated unambiguously to an arbitrarily high order, the same algorithm as presented in this paper is applicable to any integral equation of similar type, for instance, the Blankenbecler-Sugar or other similar equations.[8]

As usual, we set for the energy E of the system

$$E=k^2, \tag{2.1}$$

where k is the corresponding linear momentum. The Riccati-Bessel and Riccati-Neumann functions will be denoted by $u_l(kr)$ and $v_l(kr)$, respectively,[9] where l is the angular momentum of the partial wave. We work on the standing-wave version of the T-matrix theory and employ the standing-wave Green's function $G^{(0)}(r,r')$,

$$G^{(0)}(r,r')=k^{-1}u_l(kr_<)v_l(kr_>) . \tag{2.2}$$

The standing-wave version of scattering theory has a mathematical merit in that any variable may be taken to be real; this is particularly convenient to envision the behavior of the wave function in a close-collision state.[4] On the other hand, many aspects of physics of collision processes may be described straightforwardly by the outgoing-wave version; it will be discussed only briefly in Appendix B of the present paper, and its relation with the standing-wave version will be left for a future work.

To simplify the notation, the free-wave (inhomogeneous) term in the Lippmann-Schwinger equation will be denoted by ϕ_f, instead of $u_l(kr)$,

$$\phi_f(r)\equiv u_l(kr) . \tag{2.3}$$

Let the potential in the ordinary sense be $\underline{V}$. Let us denote the potential strength by λ and, with its use, we set

$$(r|\,V\,|r')=\lambda(r|\,v\,|r') . \tag{2.4}$$

Hereafter, $\underline{v}$ will be called the shape matrix. If the potential $\underline{V}$ is local, the shape matrix takes the form

$$(r|\,v_{\rm loc}\,|r')=v(r)\delta(r-r') , \tag{2.5}$$

where $v(r)$ is the shape function of local potential.

Hereafter we limit ourselves to a particular partial wave at a particular energy. We start from the partial-wave Lippmann-Schwinger (LS) equation

$$\psi(r)=\phi_f(r)+\lambda\int\int dr'dr''G^{(0)}(r,r')\times(r'|\,v\,|r'')\psi(r'') , \tag{2.6}$$

where k and l have been suppressed and (2.3) has been used. The asymptotic forms of the Riccati-Bessel and Riccati-Neumann functions are

$$u_l(kr)\approx\sin(kr-\tfrac{1}{2}l\pi) , \tag{2.7a}$$

$$v_l(kr)\approx-\cos(kr-\tfrac{1}{2}l\pi) , \tag{2.7b}$$

respectively.[9] It follows straightforwardly from the definition of $G^{(0)}$, (2.2), that the asymptotic form of the RHS of (2.6) is

$$\psi(r)\approx\sin(kr-\tfrac{1}{2}l\pi)+\tan\delta\cos(kr-\tfrac{1}{2}l\pi) , \tag{2.8}$$

where the tangent of the phase shift δ is defined by

$$\tan\delta=-(\lambda/k)\int\int dr\,dr'\phi_f(r)(r|\,v\,|r')\psi(r') . \tag{2.9}$$

Next, we go back to Eqs. (2.4) and (2.5) to discuss the sign of the potential. We call a shape function v of a local potential simple if it is of a single sign. We stipulate that, if v is simple, the sign of v is negative; that is, we choose an attractive potential as the standard form of a simple potential. With this sign convention for v, a bound state produced by a simple potential is associated with a certain positive value of λ in

the inhomogeneous LS equation (2.12) below. If $v(r)$ is a composite system, consisting of two parts of opposite signs, there are two sequences of bound states, one associated with positive λ and the other with negative λ. As the convention for a composite potential, we choose the sign of $v(r)$ such that the first bound state at zero energy (or zero-energy resonance for $l=0$) is associated with a positive λ, i.e., $\lambda_1>0$. The sign of a nonlocal shape matrix $\underline{v}$ may be discussed in terms of the sign of the eigenvalue λ_n in (2.12), and the sign convention for a nonlocal potential is similar to the above-stated rule for a local potential.

Consider the special values of the phase shift

$$\delta_n=(n-\tfrac{1}{2})\pi, \quad n=1,2,\ldots . \tag{2.10a}$$

These values are concerned with the attraction effect produced by a potential. First, let energy E take some negative value. According to the above-discussed sign convention of a potential, any potential has an attractive part. Hence, by adjusting the magnitude of potential strength λ, we can find a series of bound states that are associated with the respective eigenvalue λ_n of (2.12). Subsequently, we vary the energy E from negative to positive values, and continue each bound state as a function of E. The attraction effect in scattering is the continuation through positive E of the same kind of effect as forms a bound state when E is negative; and each λ_n behaves as a continuous function of E. Since the magnitude of the phase shift grows with increasing magnitude of λ, we can find a suitably large magnitude of λ with which the condition of (2.10a) may be satisfied for each applicable value of n.

Next, consider the special values of the phase shift

$$\delta_n=(n+\tfrac{1}{2})\pi, \quad n=-1,-2,\ldots . \tag{2.10b}$$

While no repulsive potential can produce any bound state ($E<0$), we must examine the effect of a repulsive potential on a scattering state ($E>0$). Even if a potential is simple, the repulsion effect that occurs for real negative λ may become so large that one of the conditions of (2.10b) becomes applicable. To see the last point, let us examine the example of a square-well potential.[10] If a repulsive square barrier is made infinitely high, namely, if λ tends to negative infinity, it becomes a hard-core potential. The hard-core phase shift remains between zero and $-\frac{1}{2}\pi$ until k becomes as large as $\pi/2$ divided by the hard-core radius. This means that there is no value of λ with which the condition of (2.10b) may be satisfied in the above range of k. However, there are a finite number of negative λ values with which the condition of (2.10b) may be satisfied, if k is larger than the limit given above. If a potential has a continuously decreasing tail, tending to zero as r tends to infinity, the repulsion effect in scattering may start at zero energy.

Let the wave function be ψ_n when one of the conditions of (2.10a) or (2.10b) is satisfied. The particular value of integer n is the radial quantum number. The relative weight of the second term on the RHS of (2.8) becomes infinitely larger than the first term, if δ takes a special value given by (2.10a) or (2.10b). Now, we multiply the free-wave term ϕ_f of (2.6) by $\cos\delta$ to change the normalization of ψ, and consider the resultant ψ as a continuous function of linear momentum k. Such an analysis will establish that the asymptotic form of ψ_n is

$$\psi_n(r)\approx A_n\cos(kr-\tfrac{1}{2}l\pi), \quad \text{as } r\to\infty , \tag{2.11}$$

where A_n is some constant. Hence, under the conditions (2.10a) or (2.10b), the wave function ψ_n satisfies the homogeneous LS equation

$$\psi_n(r)=\lambda_n\int\int dr'dr''G^{(0)}(r,r')(r'|v|r'')\psi_n(r'') . \tag{2.12}$$

A solution of the homogeneous LS equation exists if and only if λ becomes equal to λ_n, which is associated with one of the conditions given either by (2.10a) or (2.10b).

The above-mentioned special value of λ will be referred to as the λ eigenvalue hereafter. Let us first examine the λ eigenvalue for a simple potential more closely, and examine a composite potential later. The conditions listed in (2.10a) are satisfied when the associated λ eigenvalue is positive,

$$\lambda_n=|\lambda_n|>0, \quad n=1,2,3,\ldots . \tag{2.13}$$

More specifically, each λ_n is associated with the respective value of the phase shift so that

$$\lambda=\lambda_n, \quad \text{when } \delta=(n-\tfrac{1}{2})\pi . \tag{2.14}$$

The conditions of (2.10b) are satisfied if λ takes on one of the negative eigenvalues

$$\lambda_n=-|\lambda_n|<0, \quad n=-1,-2,\ldots , \tag{2.15}$$

or more specifically

$$\lambda=\lambda_{-m}, \quad \text{when } \delta=-(m-\tfrac{1}{2})\pi \text{ and } n=-m . \tag{2.16}$$

Since the magnitude of the phase shift increases with increasing magnitude of λ, the λ eigenvalues may be arranged in ascending order so that

$$\cdots<\lambda_{-2}<\lambda_{-1}<0<\lambda_1<\lambda_2<\lambda_3<\cdots . \tag{2.17}$$

In order to see the general trend for a composite potential, let us examine, as an example, a

combination of two square potentials of opposite signs. It is helpful to imagine that the results of analyzing this problem will be presented in the form of a graph that shows the behavior of each λ_n as a continuous function of energy. We begin with a system in which a square well with substantial depth is combined with a low square barrier. We determine the λ eigenvalues separately for the square well and the low square barrier. Also, we determine each λ_n directly for the composite potential, and compare it with the λ eigenvalues for the separate components. For the separate barrier, λ_m is the factor by which its height must be multiplied in order that the condition of (1.10b), for the given negative integer m, may be satisfied; the λ_m thus determined is positive. Any λ_n determined for the composite potential follows closely the pattern shown by the λ eigenvalue of the separate square well in most parts of the graph. However, in the regions where a curve representing λ eigenvalue of a square well crosses a curve representing an eigenvalue of low square barrier, the λ_n for the composite potential produces a pattern of avoided crossing. In the same manner, the λ_m, which represents the repulsion effect of the composite potential and is labeled by a negative integer, follows closely the pattern shown by the λ eigenvalue of the separate square barrier in most parts of the graph, except that we exclude the regions of avoided crossing pattern. For a stronger barrier, we gradually increase its height relative to a fixed depth of the square well. The conclusion of the analysis of the above kind is that the general rule regarding the λ eigenvalue, which has been described for a simple potential with the help of Eqs. (2.13)–(2.17), will be found equally applicable to a composite system consisting of two square potentials of opposite signs. We may assume that the same conclusion may be reached for any composite potential.

It is crucially important to the T-matrix theory that two eigenfunctions, ψ_n and ψ_m, associated with two different eigenvalues, λ_n and λ_m, respectively, are orthogonal in a functional space which is defined by using the shape matrix $\underline{v}$ as the metric operator

$$\int\int dr\,dr'\psi_m^*(r)(r|v|r')\psi_n(r')=0, \quad \text{if } \lambda_m\neq\lambda_n . \tag{2.18}$$

This result follows from the homogeneous LS equation (2.12). It is further discussed in Appendix A for the standing-wave version of the T-matrix theory, and in Appendix B for the outgoing-wave version.

Since it is shorter, we propose to refer to the T matrix of the standing-wave version as the C matrix, where the letter C has been chosen to remind us of close-collision states. Thus, the partial-wave C matrix satisfies the T-matrix equation

$$(r|C|r')=(r|V|r')+\lambda\int\int dr''dr(r|v|r'')G^{(0)}(r'',r)\times(r|C|r') . \tag{2.19}$$

The partial-wave K matrix is the on-shell part of the partial-wave C matrix

$$K(E)=(2/\pi)\int\int dr\,dr'\phi_f(r)(r|C|r')\phi_f(r') . \tag{2.20}$$

The partial-wave C matrix is related to the tangent of the phase shift by

$$\tan\delta=-k^{-1}\int\int dr\,dr'\phi_f(r)(r|C|r')\phi_f(r')=-(\pi/2k)K(E) . \tag{2.21}$$

The T-matrix equation (2.19), considered to be a linear integral equation for a fixed r', has an asymmetric kernel

$$(r|B|r')=\int dr''(r|v|r'')G^{(0)}(r'',r') . \tag{2.22}$$

We call it the rescattering operator and denote it by $\underline{B}$, where the letter B has been chosen to remind us that it raises the order in the Born expansion by one. The T-matrix equation (2.19) may be rewritten formally as

$$\underline{C}=\underline{V}+\lambda\underline{B}\underline{C} . \tag{2.23}$$

The solution $\underline{C}$ of the above equation may be set in the form

$$\underline{C}=(1-\lambda\underline{B})^{-1}\underline{V} . \tag{2.24}$$

We now introduce a function σ_n,

$$\sigma_n(r)=\int dr'(r|v|r')\psi_n(r') . \tag{2.25}$$

By multiplying $\underline{v}$ on both sides of (2.12) we see that

$$\int dr'(r|B|r')\sigma_n(r')=\eta_n(r) , \tag{2.26}$$

where

$$\eta_n=\lambda_n^{-1} . \tag{1.2}$$

Therefore, σ_n is an eigenfunction of $\underline{B}$ associated with the eigenvalue η_n. By operating $G^{(0)}$ on both sides of (2.25) and taking into account (2.12), we obtain

$$\int dr' G^{(0)}(r,r')\sigma_n(r') = \eta_n \psi_n(r) . \tag{2.27}$$

For the sake of convenience of later discussions, let us denote by $\underline{K}$ the kernel of the LS equation (2.6)

$$(r|K|r') = \int dr'' G^{(0)}(r,r'')(r''|v|r') . \tag{2.28}$$

We call it the LS kernel. In terms of $\underline{K}$, the homogeneous LS equation (2.12) may be rewritten as

$$\int dr'(r|K|r')\psi_n(r') = \eta_n \psi_n(r) , \tag{2.29}$$

hence, ψ_n is an eigenfunction of the LS kernel $\underline{K}$ associated with the same eigenvalue η_n. Both kernels $\underline{B}$ and $\underline{K}$ are a product of the Green's function $\underline{G}^{(0)}$ and the shape matrix $\underline{v}$ and asymmetric; however, they differ in the order in which the two factors are multiplied.

It is convenient to normalize ψ_n according to

$$\int\int dr\, dr' \psi_n^*(r)(r|v|r')\psi_n(r') = \mathrm{sgn}(-\eta_n) , \tag{2.30}$$

where sgn denotes the signature. Hereafter, when the complex conjugate ψ^* of the wave function ψ stands on the left-hand side, as is usual in quantum mechanics, we employ the bracket notation with use of a parentheses. Thus, we abbreviate (2.30) as

$$(\psi_n, \underline{v}\psi_n) = \mathrm{sgn}(-\eta_n) . \tag{2.30a}$$

By referring to (2.13) and (2.15), we see that the RHS of (2.30a) is positive (negative) when we deal with the repulsion (attraction) effect caused by $\underline{v}$. Also, it is convenient to define the adjoints $\psi_n^\dagger$ and $\sigma_n^\dagger$, respectively, of ψ_n and σ_n according to

$$\psi_n^\dagger(r) = \mathrm{sgn}(-\eta_n)\psi_n^*(r) \tag{2.31a}$$

and

$$\sigma_n^\dagger(r) = \mathrm{sgn}(-\eta_n)\sigma_n^*(r) . \tag{2.31b}$$

Combining the orthogonality relation (2.18) and the normalization condition (2.30), and expressing the result in terms of the adjoint, we have

$$\int\int dr\, dr' \psi_m^\dagger(r)(r|v|r')\psi_n(r') = \delta_{mn} . \tag{2.32}$$

Hereafter, when the adjoint $\psi^\dagger$ of ψ stands on the left side, we shall employ the bracket notation in which we use angular brackets. Thus, we abbreviate (2.32) as

$$\langle \psi_m, \underline{v}\psi_n \rangle = \delta_{mn} . \tag{2.32a}$$

Referring to (2.25) and (2.31a)–(2.31b), we obtain from (2.32)

$$\langle \psi_m, \sigma_n \rangle = \langle \sigma_m, \psi_n \rangle = \delta_{mn} . \tag{2.33}$$

It follows from (2.27) and (2.33) that

$$\langle \sigma_m, \underline{G}^{(0)}\sigma_n \rangle = \eta_n \delta_{mn} . \tag{2.34}$$

We refer to (2.32a) as the ψ-space orthonormal relation, reminding ourselves that the common notation for the wave function in quantum mechanics is ψ. On the other hand, as is clear from (2.38) below, the set of $\sigma_n(r)$ will be available as the basis of functional space, if we want to analyze the matrix element $(r|C|r')$ of the C matrix as a function of r, for a fixed r'. Accordingly, we refer to (2.34) as the C-space orthonormal relation, whereas (2.33) will be referred to as the space-crossing orthonormal relation. The metric of the ψ (C) space is $\underline{v}$ ($\underline{G}^{(0)}$).

Suppose we include a number L of the repulsion effect eigenfunctions (negative λ and quantum number) and a number M of the attraction effect eigenfunctions (positive λ and quantum number) to develop a finite-rank approximation. Let the sum of L and M be N,

$$N = L + M . \tag{2.35}$$

We now set, for the shape matrix $\underline{v}$,

$$(r|v|r') = \sum_{n=-L}^{+M} \sigma_n(r)\sigma_n^\dagger(r') + (r|R^{[N]}|r') , \tag{2.36}$$

where $\underline{R}^{[N]}$ is the residual term, which will be discarded if we decide to use the rank-N approximation. In order to satisfy the homogeneous LS equation (2.29) at any spectral point of λ that is included in the rank-N approximation, i.e.,

$$\lambda = \lambda_n, \quad -L \leq n \leq +M, \quad n \neq 0 ,$$

the residual term $\underline{R}^{[N]}$ of (2.36) must satisfy the condition

$$\int dr'(r|R^{[N]}|r')\psi_n(r') = 0, \quad -L \leq n \leq +M . \tag{2.37}$$

The above condition can be verified easily by using the space-crossing orthonormal relation (2.33). By using the form given by (2.36) for $\underline{v}$ on the RHS of (2.24), we obtain for the C matrix

$$(r|C|r') = \lambda \sum_{n=-L}^{+M} (1 - \lambda\eta_n)^{-1}\sigma_n(r)\sigma_n^\dagger(r') + (r|\rho^{[N]}|r') , \tag{2.38}$$

where $\underline{\rho}^{[N]}$ is the residual part of the C matrix that takes into account the effect caused by the residual part $\underline{R}^{[N]}$ of the potential. By combining the results of (2.38) and (2.20), and comparing with (1.1), we find that the residue parameter S_n of (1.1) is given by

$$S_n = (2/\pi)(\phi_f, \sigma_n)\ \langle \sigma_n, \phi_f \rangle . \tag{2.39}$$

If the decomposition of the shape matrix $\underline{v}$ into separable factors is continued indefinitely, we should obtain

$$\langle r|R^{[N]}|r'\rangle = \sum_{n<-L} \sigma_n(r)\sigma_n^\dagger(r') + \sum_{n>M} \sigma_n(r)\sigma_n^\dagger(r') \,. \tag{2.40}$$

Then, the condition of (2.37) may be easily proved on the basis of the space-crossing orthonormal relation (2.33). The rank-N approximation of the C matrix, (2.38), clearly shows that, when the matrix element $\langle r|C|r'\rangle$ is considered to be a function of r [r'], it may be expanded in a series of $\sigma_n(r)$ [$\sigma_n^\dagger(r')$].

The finite-rank approximation of the C matrix, shown above, may converge to the exact C matrix in the limit as the rank N tends to infinity. Under certain conditions that are approximately sufficient to remove a strong singularity or a long-range tail of the interaction potential, a convergence proof was worked out in momentum space in Ref. 3, based on Weierstrass's approximation theorem.[11] If we limit ourselves to a simple local potential and to the zero-energy limit of the S-wave scattering, $E=l=0$, we may discuss the basis for the finite-rank approximation in an appealing way.[12] The condition that a local potential be free from a strong singularity and from a long-range tail is that there exists an integral[9]

$$\int_0^\infty dr\, r|v(r)| < \infty \,. \tag{2.41}$$

Then, there exists a well-defined function s of r,

$$s(r) = \int_0^r dr' |v(r')|^{1/2} , \tag{2.42}$$

for any r, $0 \le r \le \infty$. In particular, as r tends to infinity $s(\infty)$ takes a finite value. As r varies from zero to infinity, $s(r)$ increases monotonically and maps an infinite range of r into a finite range of s. Therefore, one may obtain the Fourier series representation of the δ function of $s(r) - s(r')$,

$$\delta(s(r)-s(r')) = [2/s(\infty)]\sum_{n=1}^{\infty} \sin[n\pi s(r)/s(\infty)] \times \sin[n\pi s(r')/s(\infty)] \,. \tag{2.43}$$

When we re-express the δ function $\delta(r-r')$ on the RHS of (2.5) with use of $\delta(s(r)-s(r'))$ of (2.43), we obtain a series expansion of the shape matrix of a simple local potential

$$\langle r|v_{\rm loc}|r'\rangle = -|v(r)|\,\delta(r-r') = -\sum_{n=1}^{\infty} f_n(r) f_n(r') \,, \tag{2.44}$$

where the nth member of the series is constructed by using the form factor

$$f_n(r) = [2/s(\infty)]^{1/2} |v(r)|^{3/4} \sin[n\pi s(r)/s(\infty)] \,. \tag{2.44a}$$

The form factor $f_n(r)$ for large quantum number n is close to the C-space eigenfunction, as may be shown with the help of the WKB approximation,[13]

$$f_n(r) \simeq \sigma_n(r), \quad n \gg 1 \,. \tag{2.45}$$

One can also exactly solve, for $E=l=0$, three examples:

$$|v(r)| = \exp[-(r/a)], \quad (a+r)^{-4}, \quad \text{or} \quad (a^2+r^2)^{-2}$$

where a is a certain range parameter, and one can verify directly that the asymptotic statement of (2.45) is true.

Summarizing, we have dealt with two asymmetric kernels, $\underline{K}$ of (2.28) and $\underline{B}$ of (2.22). The eigenfunctions of these two kernels are related to each other, as shown in (2.25) and (2.27), but each kind is more useful than the other for particular purposes. The physical meaning of the eigenfunctions and the associated eigenvalues may be readily understood for the kernel $\underline{K}$, and its details are discussed with the help of Eqs. (2.10a)–(2.17). An eigenfunction of $\underline{K}$ is referred to as a ψ-space eigenfunction, and if it is normalized according to (2.30), the resultant rank-N approximation of $\underline{v}$ takes the simple form shown in (2.36). On the other hand, an eigenfunction of the kernel $\underline{B}$, called the C-space eigenfunction, is directly useful to write down the C matrix in the form given by (2.38). Eigenfunctions of each type span a functional space which is defined by using a metric of its kind, as shown by (2.32) and (2.34). For certain calculations, the space-crossing orthonormal relations (2.33) are very useful. The fact that, as far as the T-matrix theory is concerned, a discrete set $\{\sigma_n\}$ serves as a complete set for the eigenfunction expansion of the C matrix (at each E and l) is a consequence of the condition that $\underline{v}$ is free from a strong singularity or a long-range tail.

III. THE C-SPACE BASIS GENERATED BY ITERATION OF THE LIPPMANN-SCHWINGER KERNEL

Let us start from the free-wave term of the LS equation (2.6) and iterate the LS kernel $\underline{K}$ to generate a series of functional bases $\{\phi_n; n=1,2,\ldots\}$. The $(n+1)$th member is related to the nth member by a recurrence relation

$$\phi_{n+1}(r) = \int dr' \langle r|K|r'\rangle \phi_n(r') \,, \tag{3.1}$$

where $\underline{K}$ is the LS kernel, (2.28). The first member $\phi_1(r)$ is the free-wave term

$$\phi_1(r) = \phi_f(r) . \tag{3.2}$$

The formal Born series of the solution ψ of the LS equation (2.6) may be written as

$$\psi(r) = \sum_{n=1}^{\infty} \lambda^{n-1} \phi_n(r) . \tag{3.3}$$

The Born expansion of the tangent of phase shift may be obtained by substituting the RHS of (3.3)in place of ψ on the RHS of (2.9). Also, recall (2.21) as well as (1.3). The obtained result reads

$$\int\int dr\, dr' \phi_f(r)(r|v|r')\psi(r') = (\pi/2)K(E) = \sum_{n=1} \lambda^n K_n , \tag{3.4}$$

where

$$K_n = (\phi_1, \underline{v}\phi_n) = (\phi_n, \underline{v}\phi_1) . \tag{3.5}$$

Since we are dealing with the standing-wave version, all ϕ_n's as well as all K_n's are real. Note that the general formula

$$(\phi_m, \underline{v}\phi_n) = (\phi_n, \underline{v}\phi_m) = K_{n+m-1} \tag{3.6}$$

holds for any n and m.

We also introduce a series of functions

$$\theta_n(r) = \int dr'(r|v|r')\phi_n(r') , \tag{3.7}$$

to expand the shape matrix $\underline{v}$. Our main problem is to examine whether the functional basis $\{\theta_n; n = 1, 2, \ldots\}$ serves as a complete basis for expanding the C matrix. As shown by (2.38), the C matrix may be expanded in the C-space eigenfunctions σ_n and their adjoints $\sigma_n^\dagger$. Also, we may assume the convergence of the finite-rank approximation, and hence we may assume that, upon replacing N of (2.38) with M, the residual term $\underline{\rho}^{[M]}$ becomes small for a sufficiently large M. Therefore, if the answer to our problem is going to be affirmative, we ought to be able to show that the first M C-space eigenfunctions σ_m, $m = 1, 2, \ldots, M$, may be closely approximated by a suitable linear combination of the first N members, say of the $\{\theta_n\}$ set, or

$$\left| \sigma_m(r) - \sum_{n=1}^{N} a_{nm} \theta_n(r) \right| < \epsilon, \quad m = 1, 2, \ldots, M , \tag{3.8}$$

where ϵ is a small parameter to set an error bound and a_{nm}'s are suitable coefficients of linear combination. Although the results obtained in Sec. IV are not explicitly stated in a form similar to (3.8), the conclusion reached there gives, in restatement, an affirmative answer to our main problem

Since the $\{\phi\}$ set is not orthonormalized, we first carry out the Schmidt orthogonalization and normalization of the $\{\phi\}$ set. The functional nature of the ϕ space is the same as the ψ space. Hence, we employ the metric $\underline{v}$ in defining the orthonormal relation, as instructed by (2.32). The new basis obtained after the orthonormalization will be denoted by χ_n, which is a linear combination of ϕ_j

$$\chi_n = \sum_{j=1}^{N} \phi_j b_{jn}, \quad n = 1, 2, \ldots, N . \tag{3.9}$$

The coefficients b_{jn} should be chosen in such a way that the conditions

$$\int\int dr\, dr' \chi_m^\dagger(r)(r|v|r')\chi_n(r') = \delta_{mn}, \quad m, n = 1, 2, \ldots, N , \tag{3.10}$$

may be satisfied among the members of the $\{\chi\}$ set.

We denote by Δ_n a determinant[14]

$$\Delta_n = \begin{vmatrix} K_1 & K_2 & \cdots & K_n \\ K_2 & K_3 & \cdots & K_{n+1} \\ \cdots & \cdots & \cdots & \cdots \\ K_n & K_{n+1} & \cdots & K_{2n-1} \end{vmatrix} . \tag{3.11}$$

For the first two special cases, we stipulate that

$$\Delta_0 = 1 \tag{3.12a}$$

and

$$\Delta_1 = K_1 . \tag{3.12b}$$

We denote by $\Delta_{n,\alpha}$ a related determinant, in which a substitution $K_i \to K_{i+1}$, i.e., the raising of order in the Born expansion by one, is performed on all elements of the last α rows. For example, for $n = 2$, we have

$$\Delta_{2,0} = \Delta_2 = \begin{vmatrix} K_1 & K_2 \\ K_2 & K_3 \end{vmatrix} , \tag{3.13a}$$

$$\Delta_{2,1} = \begin{vmatrix} K_1 & K_2 \\ K_3 & K_4 \end{vmatrix} , \tag{3.13b}$$

and

$$\Delta_{2,2} = \begin{vmatrix} K_2 & K_3 \\ K_3 & K_4 \end{vmatrix} . \tag{3.13c}$$

The new bases $\chi_n(r)$ that satisfy the conditions of (3.10) will be given by

$$\chi_n(r)=|\Delta_n\Delta_{n-1}|^{-1/2}\sum_{i=1}^{n}(-1)^{i-1}\Delta_{n-1,i-1}\phi_{n-i+1}(r)$$

$$=|\Delta_n\Delta_{n-1}|^{-1/2}\begin{vmatrix} K_1 & K_2 & \cdots & \phi_1 \\ K_2 & K_3 & \cdots & \phi_2 \\ \cdots & \cdots & \cdots & \cdots \\ K_n & K_{n+1} & \cdots & \phi_n \end{vmatrix} . \quad (3.14)$$

The determinant shown above is similar to Δ_n shown in (3.11), but its nth column is replaced with a column of $\{\phi_i; i=1,2,\ldots,N\}$. The adjoint $\chi_n^\dagger$ is defined by

$$\chi_n^\dagger(r)=\mathrm{sgn}(\Delta_n\Delta_{n-1})\chi_n(r) . \quad (3.15)$$

The proof of (3.14) and (3.15) proceeds as follows. By using (3.6) and the second member of (3.14), and letting m run from 1 through $n-1$, we obtain

$$(\phi_m,\underline{v}\chi_n)=|\Delta_n\Delta_{n-1}|^{-1/2}\sum_{i=1}^{n}(-1)^{i-1}\Delta_{n-1,i-1}K_{m+n-i}$$

$$=|\Delta_n\Delta_{n-1}|^{-1/2}\begin{vmatrix} K_1 & K_2 & \cdots & K_{n-1} & K_m \\ K_2 & K_3 & \cdots & K_n & K_{m+1} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ K_n & K_{n+1} & \cdots & K_{2n-2} & K_{m+n-1} \end{vmatrix}$$

$$=0, \quad m=1,2,\ldots,n-1 . \quad (3.16)$$

In (3.16), m is less than n, and according to (3.14) and (3.15), any $\chi_m^\dagger$ for which m is less than n is a linear combination of ϕ_k, where k is less than n. Thus, we obtain the following orthogonality relation, for any m less than n,

$$\langle\chi_m,\underline{v}\chi_n\rangle=0, \quad n>m , \quad (3.17)$$

which has been written in the notation of (2.32) and (2.32a). Similarly, in analogy to (3.16) one easily obtains

$$\langle\chi_n,\underline{v}\phi_m\rangle=0, \quad m=1,2,\ldots,n-1 . \quad (3.16a)$$

By using (3.6), the second member of (3.14), (3.15), and (3.16a), it follows that

$$\langle\chi_n,\underline{v}\chi_m\rangle=0, \quad n>m . \quad (3.17a)$$

Hence, by combining (3.17) and (3.17a) it follows that the orthogonality relation in (3.10) holds for any m which is not equal to n. If m in (3.16) becomes equal to n we obtain

$$(\phi_n,\underline{v}\chi_n)=\mathrm{sgn}(\Delta_n)\,|\Delta_n/\Delta_{n-1}|^{1/2} . \quad (3.18)$$

Analogously, if m in (3.16a) becomes equal to n we obtain

$$\langle\chi_n,\underline{v}\phi_n\rangle=\mathrm{sgn}(\Delta_{n-1})\,|\Delta_n/\Delta_{n-1}|^{1/2} . \quad (3.18a)$$

By using the second member of (3.14), (3.16a), and (3.18a), we obtain the normalization of χ_n

$$\langle\chi_n,\underline{v}\chi_n\rangle=1 . \quad (3.19)$$

This concludes the proof that the new basis $\{\chi_n\}$, defined by (3.14) and (3.15), satisfies the orthonormalization dictated by (3.10).

Next, we will examine how useful the rank-N approximation of the shape matrix $\underline{v}$ based on the $\{\chi_n\}$ set is. The formulas (2.25) and (2.36) suggest that we should build separable potentials with use of the form factors $\xi_n(r)$ and their adjoints $\xi_n^\dagger(r)$, which are defined by

$$\xi_n(r)=\int dr'(r|v|r')\chi_n(r') \quad (3.20)$$

and

$$\xi_n^\dagger(r)=\int dr'\chi_n^\dagger(r')(r'|v|r) . \quad (3.21)$$

Employing the notations of (3.7), (3.14), and (3.15), the above quantities may be written as

$$\xi_n(r)=|\Delta_n\Delta_{n-1}|^{-1/2}\sum_{i=1}^{n}(-1)^{i-1}\Delta_{n-1,i-1}\theta_{n-i+1}(r) \quad (3.22)$$

and

$$\xi_n^\dagger(r)=\mathrm{sgn}(\Delta_n\Delta_{n-1})\xi_n(r) . \quad (3.23)$$

The simplest shape matrix of rank N which we can build with the use of these form factors is

$$(r|\Pi^{[N/N]}|r')=\sum_{n=1}^{N}\xi_n(r)\xi_n^\dagger(r') . \quad (3.24)$$

We will show in the next section that the above shape matrix reproduces the $[N/N]$ Padé approximant.

IV. CALCULATION OF THE K MATRIX FOR THE RANK-N POTENTIAL, (1.19)

We will first determine the C matrix for the rank-N potential (1.19) [or (3.24)] and subsequently the K matrix. The C matrix, denoted by $\underline{C}^{[N]}$, may assume the form

$$(r|C^{[N]}|r')=\sum_{m,n=1}^{N}\xi_m(r)\Gamma_{mn}^{[N]}\xi_n^\dagger(r') . \quad (4.1)$$

To help with the calculation of the matrix $\Gamma^{[N]}$ introduced above, we define a matrix $\underline{M}^{[N]}$, whose matrix elements are

$$M_{mn}^{[N]}=\langle\xi_m,\underline{G}^{(0)}\xi_n\rangle, \quad 1\leq m,n\leq N . \quad (4.2)$$

When (3.24) and (4.1) are used for expressing $\underline{v}$ and $\underline{C}$ in (2.23), we obtain a matrix equation that involves $\underline{\Gamma}^{[N]}$

$$(\underline{1} - \lambda \underline{M}^{[N]})\underline{\Gamma}^{[N]} = \lambda \underline{1} . \tag{4.3}$$

Solving (4.3) for $\underline{\Gamma}^{[N]}$, we obtain

$$\underline{\Gamma}^{[N]} = \lambda(\underline{1} - \lambda \underline{M}^{[N]})^{-1} . \tag{4.4}$$

By using (4.4) and (4.1), the full expression for the C matrix matrix becomes

$$(r|C^{[N]}|r') = \lambda \sum_{m,n=1}^{N} \xi_m(r)(\underline{1} - \lambda \underline{M}^{[N]})^{-1}{}_{mn} \xi_n^{\dagger}(r') . \tag{4.5}$$

The K matrix, denoted by $K'^{[N]}$ to conform to the notation used in (1.14), will be given, according to (2.20), by

$$K'^{[N]} = (2\lambda/\pi) \sum_{m,n=1}^{N} (\phi_f, \xi_m)(\underline{1} - \lambda \underline{M}^{[N]})^{-1}{}_{mn} \langle \xi_n, \phi_f \rangle . \tag{4.6}$$

The formal Born series of $K'^{[N]}$, (4.6), may take a form

$$K'^{[N]} = (2/\pi) \sum_{k=1}^{\infty} \lambda^k K_k'^{[N]} . \tag{4.7}$$

By comparing the RHS of (4.7) with that of (4.6), the coefficients used in the Born expansion will be determined as

$$K_k'^{[N]} = \sum_{m,n=1}^{N} (\phi_f, \xi_m)(\underline{M}^{[N]})^{k-1}{}_{mn} \langle \xi_n, \phi_f \rangle . \tag{4.8}$$

Note that, as an immediate consequence of (3.20), we have

$$(\phi_f, \xi_m) = (\phi_1, \underline{v}\chi_m) , \tag{4.9}$$

and that the RHS of (4.9) has been evaluated in (3.16). From (3.18), (3.12a), and (3.12b), we have

$$(\phi_f, \xi_1) = \mathrm{sgn}(K_1) |K_1|^{1/2} , \tag{4.10}$$

while from (3.18a), (3.12a), and (3.12b) we obtain

$$\langle \xi_1, \phi_f \rangle = |K_1|^{1/2} . \tag{4.10a}$$

For any value of m or n other than unity, all quantities of the above type that are used on the RHS of (4.8) vanish, according to (3.16). Hence, the RHS of (4.8) may be simplified to

$$K_k'^{[N]} = K_1 (\underline{M}^{[N]})^{k-1}{}_{1,1} . \tag{4.11}$$

Next, we examine the details of the matrix $\underline{M}^{[N]}$ defined by (4.2). Recalling (3.20) and (3.21), we may rewrite the RHS of (4.2) as

$$M_{m,n}^{[N]} = \langle \chi_m, \underline{K}^{\dagger} \underline{v} \chi_n \rangle = \langle \chi_m, \underline{v} \underline{K} \chi_n \rangle , \tag{4.12}$$

where $\underline{K}$ is the LS kernel (2.28) and $\underline{K}^{\dagger}$ is its adjoint

$$(r|K^{\dagger}|r') = \int dr''(r|v|r'')G^{(0)}(r'', r') = (r|B|r') . \tag{4.13}$$

It follows from (3.14), (3.15), and (3.1) that

$$\int dr' \chi_m^{\dagger}(r')(r'|K^{\dagger}|r) = \mathrm{sgn}(\Delta_m \Delta_{m-1}) |\Delta_m \Delta_{m-1}|^{-1/2} \times \sum_{i=1}^{m} (-1)^{i-1} \Delta_{m-1,i-1} \phi_{m-i+2}(r) . \tag{4.14}$$

Thus, the RHS of (4.14) is a linear combination of ϕ_j, where j runs from 2 through $m+1$. Therefore, recalling (3.16), we may conclude that

$$M_{m,n}^{[N]} = 0, \quad \text{if } n > m+1 . \tag{4.15}$$

Similarly, we have

$$\int dr'(r|K|r')\chi_n(r') = |\Delta_n \Delta_{n-1}|^{-1/2} \sum_{i=1}^{n} (-1)^{i-1} \Delta_{n-1,i-1} \phi_{n-i+2}(r) . \tag{4.16}$$

Recalling (3.16a), we may then conclude that

$$M_{m,n}^{[N]} = 0, \quad \text{if } m > n+1 . \tag{4.17}$$

By combining the results of (4.15) and (4.17), we conclude that

$$M_{m,n}^{[N]} = 0, \quad \text{if } |m-n| > 1 . \tag{4.18}$$

In other words, a matrix element $M_{m,n}^{[N]}$ may not vanish only on the diagonal $m=n$, or right next to the diagonal $m = n \pm 1$.

To calculate the matrix element for $m = n-1$, note that

$$M_{n-1,n}^{[N]} = \mathrm{sgn}(\Delta_{n-1}) |\Delta_{n-2}/\Delta_{n-1}|^{-1/2} (\phi_n, \underline{v}\chi_n) , \tag{4.19}$$

which follows from the second member of (4.12), (4.14), and (3.16). Hence, recalling (3.18), we obtain

$$M_{n-1,n}^{[N]} = \mathrm{sgn}(\Delta_{n-1}) |\Delta_n \Delta_{n-2}|^{1/2} \Delta_{n-1}^{-1} . \tag{4.20}$$

Similarly, using (4.16), the last member of (4.12), (3.16a), and (3.18a), we obtain

$$M_{n,n-1}^{[N]} = \mathrm{sgn}(\Delta_{n-2}) |\Delta_n \Delta_{n-2}|^{1/2} \Delta_{n-1}^{-1} . \tag{4.21}$$

By inspection of the determinant shown in (3.16), after setting $m = n+1$, we see that

$$(\phi_{n+1}, v\chi_n) = |\Delta_n \Delta_{n-1}|^{-1/2} \Delta_{n,1} . \tag{4.22}$$

With regards to the diagonal element $M_{n,n}^{[N]}$, it follows from the second member of (4.12) and (4.14) that

$$M_{n,n}^{[N]} = \mathrm{sgn}(\Delta_n \Delta_{n-1}) |\Delta_n \Delta_{n-1}|^{-1/2} [\Delta_{n-1}(\phi_{n+1}, \underline{v}\chi_n) - \Delta_{n-1,1}(\phi_n, \underline{v}\chi_n)] . \tag{4.23}$$

Using (4.22) and (3.18), we then obtain

$$M_{n,n}^{[N]} = (\Delta_{n,1}/\Delta_n) - (\Delta_{n-1,1}/\Delta_{n-1}) . \tag{4.24}$$

We have thus determined all matrix elements

of $\underline{M}^{[N]}$ for any N. As sketched in (1.9) of the Introduction, and as shown on the RHS of (4.11), our next step might be to determine, for any N, the (1,1) matrix element of the kth power $(\underline{M}^{[N]})^k$ for all k less than $2N$, $1 \leq k \leq 2N-1$. It appears quite possible to determine the general form of $(\underline{M}^{[N]})^k_{1,1}$ by the mathematical induction. However, a part of the algebraic work to do so is not yet complete. Hence, we will turn to the special cases $N=1,2$, and 3 to demonstrate that the special rank-N potential (1.19) [or (3.24)], reproduces the $[N/N]$ Padé approximant. The general case, as much as has been completed, will be discussed subsequently.

A. Rank-one approximation

If $N=1$, there is only one member of the $\{\chi\}$ set available for building the separable potential given in (3.24), that is,

$$\chi_1(r) = |K_1|^{-1/2}\phi_f(r) \tag{4.25}$$

and its adjoint

$$\chi_1^\dagger(r) = \mathrm{sgn}(K_1)\,|K_1|^{-1/2}\phi_f(r)\,, \tag{4.25a}$$

which have been given in implicit form by (3.12a), (3.12b), and (3.14). It is easy to calculate the matrix element

$$M^{[1]}_{1,1} = \langle \chi_1, \underline{v}\,\underline{G}^{(0)}\,\underline{v}\chi_1\rangle = K_2/K_1\,. \tag{4.26}$$

Having the rank equal to one, the matrix $\underline{M}^{[1]}$ reduces to a single number, (4.26). Substituting this result for $\underline{M}^{[N]}$ on the RHS of (4.11) we obtain

$$K'^{[1]}_k = K_2^{k-1}K_1^{2-k}\,. \tag{4.27}$$

By using (4.27) on the RHS of (4.7), the Born series for the rank-one K matrix $K'^{[1]}$ may be straightforwardly summed, to give the well-known form of the $[1/1]$ Padé approximant of the original K matrix (3.4),

$$K'^{[1]} = (2\lambda/\pi)K_1[1-\lambda(K_2/K_1)]^{-1} = K^{[1/1]}\,. \tag{4.28}$$

B. Rank-two approximation

The (1,1) matrix element $M^{[2]}_{1,1}$ of $\underline{M}^{[2]}$ is the same as the result obtained for $N=1$ in (4.26). Other elements may be obtained from (4.20), (4.21), and (4.24), by setting $n=2$ in these formulas. We also need the matrix elements of the second and third powers of $\underline{M}^{[2]}$. In writing them down, we suppress the superscript [2], and the list of these matrix elements includes:

$$M^2_{1,1} = K_3/K_1\,, \tag{4.29a}$$

$$M^2_{1,2} = \Delta_{2,1}/(|\Delta_2|^{1/2}K_1), \tag{4.29b}$$

$$M^2_{2,1} = \mathrm{sgn}(\Delta_2)M^2_{1,2}\,, \tag{4.29c}$$

and

$$M^3_{1,1} = K_4/K_1\,. \tag{4.30a}$$

Let us then introduce a new formula for $K'^{[N]}$. By using (4.9), (4.10), and (4.10a) the RHS of (4.6) may be rewritten as

$$K'^{[N]} = (2\lambda/\pi)K_1[(\underline{1}-\lambda\underline{M}^{[N]})^{-1}]_{1,1}\,. \tag{4.31}$$

The specific form, which the above general formula takes for $N=2$, is

$$K'^{[2]} = P_2(\lambda)/Q_2(\lambda)\,, \tag{4.32}$$

where the numerator and the denominator are, respectively,

$$P_2(\lambda) = (2\lambda/\pi)K_1(1-\lambda M_{2,2}) = (2\lambda/\pi)K_1\{1-\lambda[(\Delta_{2,1}\Delta_2)-(K_2/K_1)]\} \tag{4.32a}$$

and

$$Q_2(\lambda) = \det(\underline{1}-\lambda\underline{M}^{[2]}) = (\Delta_2 - \lambda\Delta_{2,1}+\lambda^2\Delta_{2,2})/\Delta_2\,. \tag{4.32b}$$

The RHS of (4.32) is identical with the $[2/2]$ Padé approximant of the original K matrix (3.4) expressed as a quotient of two second-order rational functions of λ.

Therefore, the K matrix $K'^{[2]}$ for the rank-two potential $\underline{\Pi}^{[2/2]}$, (3.24), is equal to the $[2/2]$ Padé approximant of the original K matrix

$$K'^{[2]} = K^{[2/2]}\,. \tag{4.33}$$

C. Rank-three approximation

For the rank-three approximation, we have to compute a larger number of matrix elements as well as higher powers of $\underline{M}^{[3]}$ than before. To write down the result for such an extended part of the list of matrix elements, we introduce an additional notation for determinants. Let $\Delta_{n,1(\alpha)}$ denote a determinant which is related to Δ_n of (3.11) but differs from it in that a substitution $K_i \to K_{i+\alpha}$, i.e., the raising of order in the Born expansion by α, is carried out on each element of the last row. For example, for $n=2$ we have

$$\Delta_{2,1(\alpha)} = \begin{vmatrix} K_1 & K_2 \\ K_{2+\alpha} & K_{3+\alpha} \end{vmatrix}\,. \tag{4.34}$$

Among the matrix elements of the second and third powers of $\underline{M}^{[3]}$, some with small subscripts (n,m) remain the same in form as those listed in the preceding Sec. IV B. We omit the superscript [3] again and list the following matrix elements of the second power $\underline{M}^2$ as the addition to the list given by (4.29a)–(4.29c):

$$M^2_{1,3} = \mathrm{sgn}(K_1\Delta_3)\,|\Delta_3/(K_1\Delta_2)|^{1/2}\,, \tag{4.29d}$$

$$M^2{}_{3,1} = \mathrm{sgn}(K_1\Delta_2\Delta_3)M^2{}_{1,3}\,, \tag{4.29e}$$

$$M^2{}_{2,2} = (\Delta_{2,1(2)}/\Delta_2) - [(K_2\Delta_{2,1})/(K_1\Delta_2)]\,, \tag{4.29f}$$

$$M^2{}_{2,3} = \mathrm{sgn}(K_1)(\Delta_2|K_1\Delta_3|^{1/2})^{-1}(K_1\Delta_{3,1} - K_2\Delta_3)\,, \tag{4.29g}$$

$$M^2{}_{3,2} = \mathrm{sgn}(K_1\Delta_3)M^2{}_{2,3}\,. \tag{4.29h}$$

For the third power $\underline{M}^3$ we list in addition to (4.30a)

$$M^3{}_{1,2} = (K_1|\Delta_2|^{1/2})^{-1}\Delta_{2,1(2)}\,, \tag{4.30b}$$

$$M^3{}_{2,1} = \mathrm{sgn}(\Delta_2)M^3{}_{1,2}\,, \tag{4.30c}$$

$$M^3{}_{1,3} = \mathrm{sgn}(K_1)|K_1\Delta_2\Delta_3|^{-1/2}\Delta_{3,1}\,, \tag{4.30d}$$

$$M^3{}_{3,1} = \mathrm{sgn}(K_1\Delta_2\Delta_3)M^3{}_{1,3}\,, \tag{4.30e}$$

$$M^3{}_{2,2} = (\Delta_{2,1(3)}/\Delta_2) - [(K_2\Delta_{2,1(2)})/(K_1\Delta_2)]\,. \tag{4.30f}$$

The list of the matrix elements of the fourth power $\underline{M}^4$, calculated with the use of (4.30a)–(4.30f), includes

$$M^4{}_{1,1} = K_5/K_1\,, \tag{4.35a}$$

$$M^4{}_{1,2} = (K_1|\Delta_2|^{1/2})^{-1}\Delta_{2,1(3)}\,, \tag{4.35b}$$

$$M^4{}_{2,1} = \mathrm{sgn}(\Delta_2)M^4{}_{1,2}\,. \tag{4.35c}$$

We can calculate the (1,1) element of the fifth power $\underline{M}^5$, with the use of (4.35a)–(4.35c), which gives

$$M^5{}_{1,1} = K_6/K_1\,. \tag{4.36}$$

The results shown in (4.26), (4.29a), (4.30a), (4.35a), and (4.36) have established that for each power of k that runs from 1 through 5, the (1,1) element of $\underline{M}^k$ is given by

$$M^k{}_{1,1} = K_{k+1}/K_1\,, \quad k \leq 5\,. \tag{4.37}$$

Using the above result on the RHS of (4.11) we obtain

$$K'^{[3]}_k = K_k\,, \quad k \leq 6\,, \tag{4.38}$$

for the coefficients of the Born expansion of the K matrix $K'^{[3]}$ for the rank-three shape matrix $\Pi^{[3/3]}$, (3.24). On the other hand, the formula (4.6) or (4.31) implies that $K'^{[3]}$ must be a quotient of two third-order polynomials of λ.

$$K'^{[3]} = (2\lambda/\pi)K_1(1 + \lambda b_2 + \lambda^2 b_3)/(1 + \lambda a_1 + \lambda^2 a_2 + \lambda^3 a_3)$$
$$= P'_3(\lambda)/Q'_3(\lambda)\,. \tag{4.39}$$

The undetermined coefficients, a_i's and b_j's, in the second member of (4.39) may be determined uniquely by the conditions given by (4.38). The result may be presented in the form of a continued fraction

$$K'^{[3]} = \cfrac{(2\lambda/\pi)K_1}{1 - \cfrac{\lambda(K_2/K_1)}{1 - \cfrac{\lambda(\Delta_2/K_2K_1)}{1 - \cfrac{\lambda[(\Delta_{2,2}/\Delta_2K_2)K_1]}{1 - \cfrac{\lambda[(\Delta_3/\Delta_{2,2}\Delta_2)K_2]}{1 - \lambda[(\Delta_{3,3}/\Delta_3\Delta_{2,2})\Delta_2]}}}}}\,. \tag{4.40}$$

The RHS of (4.40) agrees exactly with the [3/3] Padé approximant of the original K matrix, as suggested by (1.9) while reviewing the subject in the Introduction. Thus, we have proved that

$$K'^{[3]} = K^{[3/3]}\,. \tag{4.41}$$

Incidentally, the continued fraction form of the Padé approximant has an advantage in that the coefficients determined in a lower-rank calculation remain unchanged in higher-order calculations. The general form of the coefficient may be determined by inspection of coefficients used in (4.40). According to (3.12a)–(3.13c), we have

$$\Delta_0 = \Delta_{0,0} = 1\,, \quad \Delta_1 = K_1\,, \quad \Delta_{1,1} = K_2 \tag{3.13d}$$

for the special cases of low-rank determinants. The general form of the coefficient placed at an even-numbered position is

$$\alpha_{2n} = (\Delta_{n+1}/\Delta_{n,n}\,\Delta_n)\Delta_{n-1,n-1}\,. \tag{4.42a}$$

To use (4.42a) with $n = 1$, one should refer to the list given in (3.13d). The coefficient placed at the next position (odd numbered) is

$$\xrightarrow{\text{flow:}} \quad \alpha_{2n+1} = (\Delta_{n+1,n+1}/\Delta_{n+1}\,\Delta_{n,n})\Delta_n\,. \tag{4.42b}$$

To use (4.42b) with $n = 0, 1$, one should refer to the list given in (3.13d). The type of formula adopted for (4.42a) and (4.42b) has been deliberately chosen in order to let each factor, a determinant of the type of Δ_m or $\Delta_{m,m}$, flow through the four positions in the formula from left to right, as the subscript for the coefficient α is raised successively [shown by an arrow in front of Eq. (4.42b)]; the coefficient α is a quotient of two different combinations of determinants, and the first and fourth positions in the formula are for writing down the numerator, the second and third being for writing down the denominator.[15] Such a "flow pattern" may serve as a useful mnemonic aid.

D. Discussion on the general case

In order to extend the same type of approach as given in the preceding subsection to ranks higher than three, we may try to prove a result of the form of (4.37) for the general case by

mathematical induction. We shall now discuss the prospect of such an undertaking.

We have noticed that the (1,1) element of the second power, $(M^{[N]})^2_{1,1}$, was determined in the rank-two calculation, (4.29a), but its form remained unchanged in any higher-rank calculation, $N>2$. With that example in mind, let us consider the general case. Our problem is to examine the (m,n) matrix element of the kth power $(M^{[N]})^k_{m,n}$, $1\leq m,n\leq N$, of the rank-N matrix $\underline{M}^{[N]}$. Since the matrix $\underline{M}^{[N]}$ is truncated with a size of $N\times N$, as experienced in the rank-three calculation, the effect of truncating $\underline{M}$ starts to appear as we keep raising the power k. Quantitatively, $(M^{[N]})^k_{m,n}$ depends on N if m, n, k, and N satisfy the inequality

$$m+n>2N+1-k. \tag{4.43}$$

It is implied by (4.43) that a matrix element of the N-dependent category starts to appear at the lower right-hand corner, and the N-dependent category occupies a larger portion of $(M^{[N]})^k$ if k becomes larger. In contrast, if m, n, and k are fixed, and if N grows in such a way as to reverse the direction of the above inequality, the (m,n) matrix element of the kth power remains unchanged for any larger value of the rank N, a situation described at the onset of this paragraph in a particular example. This N-independent form will be referred to as the universal large-rank form and will be denoted by $(M^{[\infty]})^k_{m,n}$ hereafter. Qualitatively, we have

$$(M^{[N]})^k_{m,n}=(M^{[\infty]})^k_{m,n},\quad \text{if } m+n\leq 2N+1-k. \tag{4.43a}$$

Based on (4.26), (4.29a), (4.30a), (4.35a), and (4.36), we conjecture that the universal large-rank form of the (1,1) matrix element is

$$(M^{[\infty]})^k_{1,1}=K_{k+1}/K_1=\Delta_{1,1(k)}/\Delta_1, \tag{4.44a}$$

with $k=2l+1$ or $2l$, and $N\geq l+1$. As is done in writing down the RHS member of the equality in (4.44a), the notations listed in (3.13d) [given right above (4.42a)] and their generalization will be used whenever it is convenient to do so. The purpose of using such a notation is to help with our guessing at the general form for an arbitrary k. Based on (4.29b) and (4.30b), as well as on (4.29c) and (4.30c), we conjecture that

$$(M^{[\infty]})^k_{1,2}=(\Delta_1|\Delta_2|^{1/2})^{-1}\Delta_{2,1(k-1)} \tag{4.44b}$$

and

$$(M^{[\infty]})^k_{2,1}=\mathrm{sgn}(\Delta_2)(M^{[\infty]})^k_{1,2}, \tag{4.44c}$$

where both (4.44b) and (4.44c) hold under the condition

$$k=2l \text{ or } 2l-1,\quad N\geq l+1.$$

Based on (4.29f) and (4.30f), we conjecture that

$$(M^{[\infty]})^k_{2,2}=(\Delta_1\Delta_2)^{-1}(\Delta_1\Delta_{2,1(k)}-\Delta_{1,1}\Delta_{2,1(k-1)}), \tag{4.44f}$$

with $k=2l-1$, $2l-2$, $N\geq l+1$. Taking some results of the rank-four calculation into account, the above list of the conjectured universal large-rank form of matrix elements may be extended. We conjecture that the following are true:

$$(M^{[\infty]})^k_{1,3}=\mathrm{sgn}(\Delta_1)|\Delta_1\Delta_2\Delta_3|^{-1/2}\Delta_{3,1(k-2)}, \tag{4.44d}$$

$$(M^{[\infty]})^k_{3,1}=\mathrm{sgn}(\Delta_1\Delta_2\Delta_3)(M^{[\infty]})^k_{1,3}, \tag{4.44e}$$

$$(M^{[\infty]})^k_{2,3}=\mathrm{sgn}(\Delta_1)(\Delta_2|\Delta_1\Delta_3|^{1/2})^{-1}\times(\Delta_1\Delta_{3,1(k-1)}-\Delta_{1,1}\Delta_{3,1(k-2)}), \tag{4.44g}$$

$$(M^{[\infty]})^k_{3,2}=\mathrm{sgn}(\Delta_1\Delta_3)(M^{[\infty]})^k_{2,3}, \tag{4.44h}$$

$$(M^{[\infty]})^k_{3,3}=(\Delta_2\Delta_3)^{-1}(\Delta_2\Delta_{3,1(k)}-\Delta_{2,1}\Delta_{3,1(k-1)}+\Delta_{2,2}\Delta_{3,1(k-2)}). \tag{4.44i}$$

Any formula among (4.44d), (4.44e), and (4.44g)–(4.44i) is valid under the condition

$$k=2l-3,\ 2l-4,\quad N>l+1.$$

It is quite possible to make a further extension of the list. For example, (4.44a), (4.44f), and (4.44i) suggest that the general form of the universal large-rank (n,n) matrix element is

$$(M^{[\infty]})^k_{n,n}=(\Delta_{n-1}\Delta_n)^{-1}\sum_{m=0}^{n-1}(-1)^m\Delta_{n-1,m}\Delta_{n,1(k-m)}. \tag{4.45}$$

However, we shall not pursue this subject any further, but leave the rest for a future work.

With the use of (4.44a)–(4.44i), we may carry out an algebraic work of the premultiplication by $\underline{M}$,

$$\underline{M}(\underline{M}^{[\infty]})^k=(\underline{M}^{[\infty]})^{k+1}, \tag{4.46a}$$

or the postmultiplication by $\underline{M}$,

$$(\underline{M}^{[\infty]})^k\underline{M}=(\underline{M}^{[\infty]})^{k+1}. \tag{4.46b}$$

Such a calculation carried out with respect to the (1,1), (1,2), (2,1), or (2,2) matrix element will enable us to verify that, when the power is raised from k to $k+1$, the same type of formula as listed in (4.44a)–(4.44c) and (4.44f) applies. The calculation is particularly simple for the (1,1) matrix element. Thus, the general proof for the universal large-rank form may be completed by mathematical induction, as far as these matrix elements are concerned. The extension of the mathematical induction proof to other matrix elements must be left for a future work.

Once the formula (4.44a) is established, that

result may be combined with (4.11) enabling us to obtain

$$K'^{[N]}_k = K_k, \quad 1 \leq k \leq 2N, \tag{4.47}$$

which is the general result applicable to an arbitrary rank N, whereas (4.38) was obtained specifically in the case of rank three. The conditions (4.47) for the Born expansion coefficients of the rank-N K matrix $K'^{[N]}$ are exactly of the same type as the analogous conditions (1.9) for the Born expansion coefficients of the $[N/N]$ Padé approximant. Hence, we obtain

$$K'^{[N]} = K^{[N,N]}, \tag{4.48}$$

which is an affirmative answer to the earlier posed question, stated in Sec. III with the help of (3.8).

V. CONCLUSIONS AND DISCUSSIONS

We have shown that one obtains the $[N/N]$ Padé approximant for the K matrix if the shape matrix $\underline{v}$, (2.4), is replaced by $\underline{\Pi}^{[N/N]}$, (3.24). That is, the approximation procedure of using the $[N/N]$ Padé approximant for the K matrix is equivalent to that of replacing the original shape matrix $\underline{v}$ by the rank-N shape matrix $\underline{\Pi}^{[N/N]}$. The possibility of obtaining this result was already discussed in 1965 by the present author.[5] In Ref. 5, we first observed that the K matrix in a rank-N problem takes the form $K'^{[N]}$, (1.14), in which one may vary $2N$ parameters S'_n and η'_n, $(n=1,\ldots,N)$, by changing the functional forms of N form factors $f_n(r)$, $(n=1,\ldots,N)$. If we successfully adjust these form factors, those $2N$ parameters may satisfy the $2N$ conditions

$$K'^{[N]}_k = \sum_{n=1}^{N} (\eta'_n)^{k-1} S'_n = K_k, \quad 1 \leq k \leq 2N. \tag{5.1}$$

The above conditions are the same as those of (4.47), but they are written down here in terms of S'_n and η'_n. Clearly, the conditions of (5.1) are sufficient to guarantee the result of (4.48). In Ref. 5, however, the concrete form of the rank-N potential that produces the desired results, (5.1), was not shown. We have completed our investigation in this paper by explicitly showing the N form factors $\xi_n(r)$, (3.22).

Once the rank-N shape matrix $\underline{\Pi}^{[N/N]}$, (3.24), is specified, any result follows, directly or indirectly, from the properties of the matrix $\underline{M}$ defined by (4.2). Our approach is based on the set of formulas (4.1)–(4.6), and straightforward. All matrix elements of $\underline{M}$ have been determined by (4.18)–(4.24). In Sec. IV D, some general discussions have been given of the kth power, $\underline{M}^k$. Three kinds of determinants have been used in writing down our results: Δ_n introduced by (3.11), $\Delta_{n,\alpha}$ explained with the help of (3.13a)–(3.13c), and $\Delta_{n,1(\alpha)}$ by (4.34). All results have been written down explicitly in terms of these kinds of determinants, thinking of convenience in application. Most parts of our algebraic work are simple; the calculations that were done to obtain the result of (3.16) are typical of such simple algebraic work. The list of notation may have to be expanded in the future. For complete determination of the kth power of the universal large-rank matrix $(\underline{M}^{[\infty]})^k$, discussed in Sec. IV D, we may need a determinant of some new type in intermediate calculations.

The simplicity of the algebra required to determine the properties of $\underline{M}$, in turn, is a consequence of the fact that the functional basis has been Schmidt orthonormalized in the ψ space at the beginning of calculation. The same result as obtained in this paper was obtained independently by Garibotti and Villani[6] for a local potential. They symmetrized the Lippmann-Schwinger kernel, (2.28), by premultiplication and postdivision by the square root of the absolute value of the shape function $|v(r)|^{1/2}$, and subsequently they used the minimal iteraction method, which is equivalent to the Schmidt orthogonalization of the basis set.[16] Their main results were given by using a certain three-term recurrence formula. To compare their results with ours, let us start from (4.31). Comparing the RHS of (4.31) with the Padé formula, (1.7), we see that the Padé numerator in the $[N/N]$ calculation should be

$$P_N(\lambda) = (2\lambda/\pi) K_1 \min_{(1,1)} [\det(\underline{1} - \lambda \underline{M}^{[N]})], \tag{5.2}$$

where $\min_{(1,1)}$ denotes the $(1,1)$ minor determinant; similarly, the $[N/N]$ Padé denominator is

$$Q_N(\lambda) = \det(\underline{1} - \lambda \underline{M}^{[N]}). \tag{5.3}$$

By inspection of the form of $\underline{M}^{[N]}$, determined by (4.18)–(4.24), we find that the three-term recurrence formula for Q_N is

$$Q_{N+1}(\lambda) = (1 - \lambda\alpha_N) Q_N(\lambda) - \lambda^2 \beta_N Q_{N-1}(\lambda), \tag{5.4}$$

where

$$\alpha_N = M_{N+1,N+1} = (\Delta_{N+1,1}/\Delta_{N+1}) - (\Delta_{N,1}/\Delta_N) \tag{5.5}$$

and

$$\beta_N = M_{N+1,N} M_{N,N+1} = \Delta_N^{-2} \Delta_{N+1} \Delta_{N-1}. \tag{5.6}$$

The initial conditions for the above three-term recurrence formula are

$$Q_0(\lambda) = 1, \quad Q_1(\lambda) = 1 - \lambda(K_2/K_1). \tag{5.4a}$$

The three-term recurrence formula for the Padé numerator $P_N(\lambda)$ is the same as for the denomi-

nator

$$P_{N+1}(\lambda)=(1-\lambda\alpha_N)P_N(\lambda)-\lambda^2\beta_N P_{N-1}(\lambda)\,, \qquad (5.7)$$

whereas the initial conditions are different, given by

$$P_0(\lambda)=0,\quad P_1(\lambda)=(2\lambda/\pi)K_1\,. \qquad (5.7a)$$

Thus, the results obtained by Garibotti and Villani may be rederived by using our alternative approach. For the special case of rank two, the results were shown in (4.32a) and (4.32b). Before passing, one may note that these results, (4.32a) and (4.32b), suggest that the explicit general formulas for $Q_N(\lambda)$ and $P_N(\lambda)$ are

$$Q_N(\lambda)=\sum_{m=0}^{N}(-\lambda)^m(\Delta_{N,m}/\Delta_N) \qquad (5.8)$$

and

$$P_N(\lambda)=(2\lambda/\pi)K_1 \times\left[1+\sum_{m=1}^{N-1}\lambda^m\sum_{i=0}^{m-1}(-1)^i(K_{m+1-i}\Delta_{N,i}/K_1\Delta_N)\right], \qquad (5.9)$$

which are well known but written down here in our notation.[17]

As for the theoretical foundation of our results, we have completely avoided the square root of the absolute value of local potential. Furthermore, instead of symmetrizing the kernel, we have dealt with the two asymmetric kernels, $\underline{B}$ of (2.22) and $\underline{K}$ of (2.28). We have used two kinds of eigenfunctions, one for each type of kernel, the C-space eigenfunctions of (2.26) and the ψ-space eigenfunctions of (2.29). As mentioned at the end of Sec. II, it is in general convenient to deal with the ψ-space eigenfunction to clarify the physical meaning of the formulas, whereas the C-space eigenfunctions are directly useful in the development of the T-matrix theory. Our approach has merit in that any interaction potential, local or nonlocal, may be dealt with as long as the kernels may be iterated to an arbitrarily higher order.

A great advantage of dealing with a finite-rank potential is that the exact wave function of the system can be obtained with little difficulty. It is easy to write down all matrix elements $\Gamma^{[N]}_{m,n}$ in (4.5), for any small value of N, such as $N=1$, 2, or 3. Hence, the off-shell T matrix may be approximated in the same spirit as the $[N/N]$ Padé approximant of the K matrix. The present method is, therefore, very useful in studying the half-shell or off-shell T matrix.[18]

An interaction potential without a long-range tail or a strong singularity has been defined in Ref. 3 in momentum space in a particular fashion. The convergence of the $[N/N]$ Padé approximant in the limit of infinite N to the exact result has also been discussed. The results of the present paper have established that, besides the sequence of finite-rank potentials based on the C-space eigenfunction (2.36), there is a second sequence of finite-rank potentials based on the Born expansion. The two sequences should become equivalent to each other, as a set, in the limit of infinite rank, but individual members are different between the two sets. At low energies, the quantum-mechanical feature of the system dominates, unless λ is large. Hence, one obtains a good approximation by retaining a relatively small number of terms in (2.36). With a rank of suitably large magnitude, one should get a good result also by employing the Padé approach presented in this paper. At high energies of the Schrödinger theory, on the other hand, each eigenfunction σ_n makes a relatively small contribution to the sum, and a large number of terms must be summed in (1.1). At the same time, all eigenvalues η_n become small in (1.1), making the Born series converge more rapidly than at lower energies. In fact, the Born series always converges in the high-energy limit of the Schrödinger theory. Thus, the finite-rank approximation based on the Padé approach of the present paper should be very useful at high and intermediate energies, whereas the finite-rank approximation based on the C-space eigenfunction may be meaningful only theoretically at high energies.

Finally, let us note that the high-energy limit is substantially different in the relativistic theory from the high-energy limit based on the Schrödinger theory. Hence, a careful examination of the relativistic two-body problem should be encouraged, keeping the results of the present paper in mind. Also, a detailed investigation into a system consisting of more than two particles should be undertaken, to extend the spirit of the present paper to areas where an improvement of the approximation method is highly desirable.

APPENDIX A: ORTHOGONALITY OF THE ψ-SPACE EIGENFUNCTION, (2.18)

Take the Hermitian conjugate of the homogeneous LS equation (2.12), after replacing the eigenvalue and eigenfunction by λ_m and ψ_m, respectively. Remember in the course of calculation that the shape matrix $\underline{v}$ is Hermitian and all other quantities are real. Then, we obtain

$$\psi^*_m(r)=\psi_m(r) =\lambda_m\int\int dr'dr''\psi_m(r'')(r''|v|r')G^{(0)}(r',r)\,. \qquad (2.12a)$$

Operating v and ψ_n from the right in succession

and integrating, we obtain

$$(\psi_m, \underline{v}\psi_n) = \lambda_m(\psi_m, \underline{v}\,\underline{G}^{(0)}\underline{v}\psi_n)\,. \tag{A1}$$

By operating v and ψ_m^* in succession from the left on both sides of (2.12) and integrating, we obtain

$$(\psi_m, \underline{v}\psi_n) = \lambda_n(\psi_m, \underline{v}\,\underline{G}^{(0)}\underline{v}\,\psi_n)\,. \tag{A2}$$

By combining (A1) with (A2), we see that

$$(\lambda_m - \lambda_n)(\psi_m, \underline{v}\,\underline{G}^{(0)}\underline{v}\,\psi_n) = 0\,. \tag{A3}$$

It follows then that if two eigenvalues are not equal,

$$(\psi_m, \underline{v}\,\underline{G}^{(0)}\underline{v}\,\psi_n) = 0, \quad \text{if } \lambda_m \neq \lambda_n\,. \tag{2.18a}$$

The result (2.18) follows from (A1) and (21.8a).

APPENDIX B: ORTHOGONALITY OF THE ψ-SPACE EIGENFUNCTION IN THE OUTGOING AND INGOING-WAVE VERSIONS

When the outgoing-wave Green's function $G^{(+)}(r, r')$ is used, the homogeneous Lippmann-Schwinger equation (2.12) becomes

$$\psi_n^{(+)}(r) = \lambda_n \int\int dr'\,dr''\,G^{(+)}(r, r')(r'|v|r'')\psi_n^{(+)}(r'')\,, \tag{B1}$$

where both the eigenvalue λ_n and the eigenfunction ψ_n are complex. Remember that the complex conjugate of $G^{(+)}$ is the ingoing-wave Green's function

$$G^{(+)}(r, r')^* = G^{(-)}(r, r')\,. \tag{B2}$$

Replacing the radial quantum number n in (B1) with m, and examining the complex conjugate, we may write down the homogeneous Lippmann-Schwinger equation of the ingoing-wave version

$$\psi_m^{(-)}(r) = \lambda_m^* \int\int dr'\,dr''\,G^{(-)}(r, r')(r'|v|r'')\psi_m^{(-)}(r'')\,, \tag{B3}$$

wherein we have assumed that the potential is real, i.e.,

$$(r'|v|r'')^* = (r'|v|r'')\,. \tag{B4}$$

The Hermitian conjugate of (B3) reads

$$\psi_m^{(-)}(r)^* = \lambda_m \int\int dr'dr''\psi_m^{(-)}(r'')^*(r''|v|r')G^{(+)}(r', r)\,. \tag{B5}$$

By operating $\underline{v}$ and $\psi_m^{(-)*}$ in succession from the left of (B1), we obtain

$$(\psi_m^{(-)}, \underline{v}\,\psi_n^{(+)}) = \lambda_n(\psi_m^{(-)}, \underline{v}\,\underline{G}^{(+)}\underline{v}\,\psi_n^{(+)})\,. \tag{B6}$$

By operating $\underline{v}$ and $\psi_n^{(+)}$ in succession from the right of (B5), we obtain

$$(\psi_m^{(-)}, \underline{v}\,\psi_n^{(+)}) = \lambda_m(\psi_m^{(-)}, \underline{v}\,\underline{G}^{(+)}\underline{v}\,\psi_n^{(+)})\,. \tag{B7}$$

By combining the results of (B6) and (B7), we obtain the biorthogonality relation that holds when two eigenvalues are not equal

$$(\psi_m^{(-)}, \underline{v}\,\psi_n^{(+)}) = 0, \quad \text{if } \lambda_m \neq \lambda_n\,. \tag{B8}$$

If we try to extend the method of eigenfunction expansion to the T-matrix theory of the outgoing wave version, the orthogonality relation of (2.18) should be replaced by the biorthogonality relation of (B8).

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