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Дискретные разложения волновых функций континуума. Общий подход

Рассмотрены различные дискретные разложения волновых функций континуума: полюсные разложения /согласно теореме Миттаг-Лефлера/, Вайнберговские состояния и т.д. Общими свойствами данных групп состояний является их полнота в конечной области пространства, они удовлетворяют уравнениям шредингеровского типа и сшиваются на границе со свободными решениями уравнения Шредингера. Исследуется сходимость разложений для S - матрицы, функций Грина и волновых функций непрерывного спектра. Вводится новая группа состояний, обладающих наилучшей сходимостью.

Работа выполнена в Лаборатории теоретической физики ОИЯИ

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Bang J. et al. E4 - 12497

Discrete Expansions of Continuum Wave Functions. General Concepts

Different methods of expanding continuum wave functions in terms of discrete basis sets are discussed. The convergence properties of these expansions are investigated, both from a mathematical and a numerical point of view, for the case of potentials of Woods-Saxon and square well type.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Communication of the Joint Institute for Nuclear Research. Dubna 1979

1. Introduction

In this article, the convergence of different expansions of single particle states in the continuum is considered.

Continuum states are met in a number of nuclear physics problems, ranging from elastic scattering, over different reactions, to calculations of nuclear structure, where the continuum states came into play in a virtual way.

In many of these cases, it is from a calculational point of view very convenient to replace the continuum functions, partly or completely, by a discrete set of states. This can be done in many ways, since essentially any complete set of functions will do; the set does not even need to be complete in all space, completeness in a final volume, which contains the nucleus, will in many calculations be sufficient.

Even this limited completeness could be disposed of in a concrete calculation, but it is a very reassuring feature of a basis, and we shall here only look at such sets, which are complete in a certain region of space, say for $r \leq a$, and more specially such sets, which satisfy equations of the Schrödinger type.

We shall further concentrate on such functions, which satisfy physical boundary conditions. This means that if the interactions (apart, possibly, from the Coulomb field) can be neglected for $r > a$, the functions are continued into solutions of the free particle (or Coulomb) Schrödinger equation. This means, that the important Green functions G^+ and G^- have simple expressions in terms of our basis functions.

We are thus excluding, e.g., the harmonic oscillator functions, the infinite well egienfunctions, and the functions of Wigner and Eisenbud /1/ used in R-matrix theory from our discussions. Since the existing literature concerning these states is very extended, we do not feel this as a serious limitation of our work.

The application of the expansion schemes discussed here, to, e.g., continuum shell model calculations, is fairly straightforward, see, e.g., /2,3,4/ and references therein. Once a discrete representation of the Green function is known, the wave functions are in general obtained by matrix inversion. Such calculations will be published elsewhere.

We shall in the next section list the main properties of the sets of functions, we are looking at. In sections 3 and 4, we shall consider the problem of using these functions as a basis of expansion in the calculation of potential scattering wave functions, as well as of the corresponding S-matrix. Although such expansions are particularly usefull in the many-channel case, with residual interactions, some of the important convergence properties are seen already for one channel with potential scattering, and we shall limit our expansion calculations to that case.

In section 3 we are looking at the Mittag-Leffler expansions /4/ mainly, whereas in section 4, we shall consider different expansions in terms of energy dependent, discrete sets of wave functions. In this connection, a new set, with particularly good convergence properties is proposed.

With a given expansion basis, a number of prescriptions can be used for the calculation of the S-matrix. These prescriptions are discussed below in connection with some concrete numerical examples.

2. Properties of the Eigenfunctions

As is said above, we shall here limit ourselves to a certain class of eigenfunction expansions, used in nuclear physics. Common to them is that the functions satisfy equations of the type

$$(H_0 + \gamma V(r) - \varepsilon)\,\psi = 0\,, \tag{2.1}$$

where $V(r) = 0$ for $r > a$. H_0 might include a Coulomb potential, but we shall here limit ourselves to the case, where it is the pure kinetic energy operator. We are looking at spherical symmetric $V's$ only, and write

$$\psi = \frac{Y_{\ell m}}{r}\,\varphi_\ell \tag{2.1a}$$

$$\left(-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + \gamma V(r) - k^2\right)\varphi_\ell(r) = 0 \qquad \left(\frac{\hbar^2}{2m}k^2 = \varepsilon\right)$$

We are particularly interested in the case, where V is the Woods-Saxon potential

$$V = \frac{V_0}{1 + \exp\frac{r-R}{\alpha}}\,.$$

This is different from 0 for all r, but if $a \gg R + \alpha$, the error by cutting off the potential at $r = a$ is negligible. When we in the following talk about a Woods-Saxon potential, we mean such a cut-off potential, and the same with the possible spin orbit term of the type

$$V_{so} \sim \frac{1}{r}\,\frac{dV}{dr}\,.$$

We shall also look at the limiting case of $\alpha \to 0$, the square well potential.

We are looking at expansions for $r \le a$ only, since we want to expand only such functions, which for $r > a$ satisfy an equation

$$(H_0 - E)\,\psi = 0 \qquad\qquad r > a \tag{2.3}$$

or, for the radial parts

$$\left(-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} - k^2\right)\Phi_\ell = 0 \qquad \left(\frac{\hbar^2}{2m}k^2 = E\right). \tag{2.3a}$$

So once the expansion for $r \le a$ is given, ψ is known for all r-values.

The basis states φ_ℓ satisfy the boundary conditions

$$\varphi_\ell(0) = 0 \tag{2.4}$$

$$\frac{d}{dr}\ln(\varphi_\ell(r)) = b , \quad r = a \tag{2.5}$$

The different sets in common use are characterized by the choices of (γ,ε) and of b, i.e., of the continuation of φ for $r>a$.

a) The bound state boundary condition is common to all the sets:

$$b = \frac{O_\ell'(k)}{O_\ell(k)} \left(= k\,\frac{h_\ell^{(+)\prime}(ka)}{h_\ell^{+}(ka)}\right) \tag{2.6a}$$

(when Coulomb field absent)

where O_ℓ is an exponentially decreasing solution of (2.3) (equal the Riccatti-Hankel function $h^+_\ell(kr)$ in the absence of Coulomb forces).

$$O_\ell \underset{r\to a}{\sim} e^{-\varkappa r} \tag{2.7}$$

characterized by the positive number

$$\varkappa = -ik , \quad E_{binding} = -\frac{\hbar^2}{2m}\varkappa^2 . \tag{2.8}$$

This means that our eigenfunction, continued as O_ℓ for $r>a$, are square integrable in all space.

We have, however, already here a choice of different eigenvalue problems, all with E,ε and γ real.

Aa) Schrödinger eigenfunctions; γ fixed, eigenvalue $\varepsilon_i = E$.

Ba) Sturm-Liouville functions; $\varepsilon = E$ fixed, eigenvalue γ_i (often called λ_i [5)])

Ca) Kapur-Peierls functions, γ, E fixed, eigenvalue $\varepsilon_i \neq E$.

The Schrödinger eigenvalue problem Aa) has for the potentials, in which we are interested, only a finite number of eigenvalues. However, the Sturm-Liouville functions, Ba) form a complete set in $\mathcal{L}_2$(a) (and this will even be the case for $a\to\infty$ /5/, and so do the Kapur-Peierls functions /6/ Ca).

For other κ values, a solution, which satisfies (2.3) will in general not be square integrable in all space, but that does not prohibit the use of similar expansions for $r \leq a$.

Here b must be chosen according to other criteria:

b) One possibility is to use again the same boundary conditions as in a), this means that our functions are obtained from those of a) by analytic continuation in k, ε and γ.

The eigenvalue problems, analogous to those listed above are then

Ab) The solutions corresponding to general poles of the S-matrix. Together with those mentioned under Aa), these form an overcomplete set for $r \leq a$ /4,7/.

Bb) The Weinberg States: $E = \varepsilon$ real >0, γ_i complex. For the potentials in which we are interested, the completeness of these states was proved /8,9/, see below.

Cb) The Usual Kapur Peierls States, E real, ε_i complex form a complete set for $r \leq a$ /6/

c) Another possibility consists in choosing real boundary conditions, also for the positive energies, i.e., φ_ℓ is for $r>a$ continued as

$$F\cos\Delta_\ell + G\sin\Delta_\ell \underset{r\to\infty}{\sim} \sin(kr + \Delta_\ell) , \tag{2.9}$$

where F_ℓ is a regular, G_ℓ an irregular solution of (2.3a), or in other words

$$b = \frac{F_\ell'\cos\Delta_\ell + G_\ell'\sin\Delta_\ell}{F_\ell\cos\Delta_\ell + G_\ell\sin\Delta_\ell} , \tag{2.6c}$$

Ac) If we use this boundary condition in the ordinary Schrödinger equation, we know that there corresponds, to each value of E, ℓ a phase shift $\delta_\ell(E)$. So we must either, for a general choice of Δ, expect to get only, at most, a few solutions $\delta_\ell(E_i) = \Delta$, or choose $\Delta_\ell(\ell, E) = \delta_\ell(E)$ in which case all positive, real E values are eigenvalues. With proper normalization, we shall in this way get the scattering states, which, together with the bound states form a complete set /10/ which, however, being continuous, falls outside the category of sets in which we are interested.

Bc) The real Weinberg states. These are usually defined with $\Delta_\ell = \frac{\pi}{2}\,(+2n\pi)$ /11,12/. This choice, which gives a simple expression for the principal value Green function, is not necessary. If we want to expand a function Ψ, which satisfies (2.3) with $E = E_0$, and has the shape given by (2.9) with $\Delta_\ell = \Delta(\ell, E_0)$, a natural choice of basis states would

be given by (2.6c) with the same $\Delta_\ell = \Delta(\ell, E_0)$.
The real Weinberg states correspond to γ_i real (often called /11,12/).

Co) The natural boundary condition states are defined as the Kapur Peierls states, but with (2.6c), where $\Delta_\ell(E)$ can again be chosen according to the function, which is to be expanded /13,14/ . Since we are here only interested in the one-channel case, we may include the eigenchannel states/13/ in Cc).

d) The Wigner-Eisenbud functions are solutions of (2.1) with a fixed, energy-independent b in (2.5). A convenient choice is $b = 0$. They form a complete orthogonal set of functions, which, however, as said above, falls outside the class of functions, in which we are interested here.

		a	b	c
square integrable		x		
exponential asymp.		x	x	
real boundary conditions		x		x
A	given γ, $\varepsilon_i = E$ eigenvalue	Schrödinger bound states	Generalized resonance states	Scattering states
B	$\varepsilon = E$ given, γ_i eigenvalue	Sturm-Liouville	(usual) Weinberg	General real Weinberg
C	γ, E given, $\varepsilon_i(\neq E)$ eigenvalue	Kapur-Peierls	(usual) Kapur-Peierls	N.B.C. et al.

In the above scheme, we have ordered the basis functions according to their main properties.

The analogy between the functions listed in line A and those of the two other lines is somewhat limited, whereas the analogy between the latter two is very close; for a square well of radius a, they are really pairwise identical, the difference being purely formal.

Note, however, that the expansions on line C depend on the radius a, whereas for a potential, as, e.g., that of Woods-Saxon, the expansions of line A and B will only depend on a through the necessary cut-off of the potential, i.e., negligibly for sufficiently large a-values.

It should be mentioned that a complete set can be constructed, using the bound states (Aa) and some of the resonances (Ab), with further inclusion of a certain continuous set of states/15/. The meaning of the completeness in Berggren's work is more general, but includes the bounded functions in $0 \le r \le a$, treated here.

Orthogonality properties and normalization

The radial functions listed under a) and c) may be chosen real; the other ones will at most be biorthogonal.

The Schrödinger bound states, Aa), together with the scattering states, Ac) are mutually orthogonal for integration over all space. If, on the other hand, we introduce the generalized resonance states, Ab) together with Aa), the generalization of the orthonormality relation of the bound states is

$$\frac{\varphi^A_{n\ell}(a)\,\varphi^A_{m\ell}(a)}{k^2_{m\ell} - k^2_{n\ell}}\left[k_{m\ell}\frac{h^+_\ell(k_{m\ell}a)'}{h^+_\ell(k_{m\ell}a)} - k_{n\ell}\frac{h^+_\ell(k_{n\ell}a)'}{h^+_\ell(k_{n\ell}a)}\right] + \int_0^a dr\, \varphi^A_{n\ell}(r)\,\varphi^A_{m\ell}(r) = \delta_{nm} \qquad (2.10)$$

which is used for the normalization of the φ's (interpreting the first term as the limit $k_n \to k_m$), but which does not have the character of an orthogonality relation. Note that the relation is independent of a, as long as $V(r) = 0$ for $r \geq a$.

The functions listed under B) are easily seen to have the orthogonality property (we shall here, and in the following omit the index ℓ)

$$\int_0^\infty \varphi^B_n(r)\, V(r)\, \varphi^B_m(r)\, dr = \delta_{nm} C_n , \qquad (2.11)$$

which can be used for normalization by putting $C_n = 1$, whereas the functions listed under C) in a similar way are orthonormalized by

$$\int_0^a \varphi^C_n(r)\, \varphi^C_m(r)\, dr = \delta_{nm} \qquad (2.12)$$

Completeness

The general pole functions (Aa + Ab) form, as mentioned above, an overcomplete set for $0 \le r < a$, since we have

$$\frac{1}{2}\sum_n \varphi_n^A(r)\,\varphi_n^A(r') = \delta(r-r'), \quad r, r' < a. \qquad (2.13)$$

This is proved from the expression for the Green function, given below [4] .

The completeness relation of the Sturm-Liouville functions (Ba), follow from Mercer's theorem [5,8], when V takes one of the forms in which we are interested (since all eigenvalues are positive). It can be written

$$\sum_n V(r)^{\frac{1}{2}}\,\varphi_n^B(r)\,\varphi_n^B(r')\,V(r')^{\frac{1}{2}} = \delta(r-r') \qquad (2.14)$$

$$\Big(=\sum_n V(r)\,\varphi_n^B(r)\,\varphi_n^B(r') = \sum_n \varphi_n^B(r)\,\varphi_n^B(r')\,V(r')\Big),$$

If we look at the expansion

$$\Psi(r) = \sum_n c_n^B\,\varphi_n^B(r) = \sum_n \varphi_n^B(r)\int \varphi_n^B(r')\,V(r')\,\Psi(r')\,dr' \qquad (2.14a)$$

this identity can be analytically continued [8] so as to get a similar relation for the usual Weinberg functions. For the real Weinberg functions, the same relation (2.14) can again be proved [16] . Here we have negative eigenvalues, but only a finite number of them [17] so Mercer's theorem is again applicable.

The three representations in (2.14) are obviously valid for slightly different classes of functions; note, however, that for the potentials in which we are interested they will all give convergent representation even for $a \to \infty$ when Ψ is a harmonic oscillator function.

The Kapur-Peierls and Natural Boundary Condition functions (C) satisfy the completeness relation

$$\sum_n \varphi_n^C(r)\,\varphi_n^C(r') = \delta(r-r'), \quad r, r' \leq a \qquad (2.15)$$

This was shown for the cases (a) and (b) in ref. [6] . In the last case, (c), the proof of Kato [16] applies again.

Mercer's theorem implies, that series like (2.14a) on the similar

$$\Psi(r) = \sum_n c_n^C\,\varphi_n^C(r) \qquad (2.16)$$

with

$$c_n^C = \int_0^a \varphi_n^C(r)\,\Psi(r)\,dr \qquad (2.17)$$

will be absolutely and uniformly convergent for the functions Ψ in which we are interested (say, any bounded function in $r \leq a$).

The corresponding expansions in terms of the pole functions (Aa+Ab) are, due to the non-orthogonality of the set, ambiguous. However, for a wide class of functions, we have an unambiguous, convergent expansion in terms of the Schrödinger eigenfunctions (Aa+Ac). On the other hand, for $r \leq a$, the scattering functions can be expanded in different, but unambiguous ways in terms of the pole functions, together with a small number of other functions, using the Mittag-Leffler theorem [4], as we shall consider in details below.

Even more important for the applications is the fact, that the single particle Green functions G^+ and G^- have simple Mittag-Leffler expansions in terms of the pole states.

<u>The Green functions</u>

The Green function G_ℓ^+ has the expansion

$$G_\ell^+(k,r,r') = \sum \frac{\varphi^A_{n(\ell)}(r)\,\varphi^A_{n(\ell)}(r')}{2k_{n(\ell)}\,(k-k_{n(\ell)})}; \quad r, r' < a \qquad (2.18)$$

in terms of the pole functions (Aa+Ab) as shown by More and Gerjuoy [18] .

Other Mittag-Leffler expansions of the Green function are

$$G_\ell^+ = \sum_{q=0}^{p}\frac{(k-k_0)^q}{q!}\,G_\ell^+(k_0,r,r')^{(q)} + \frac{(k-k_0)^{p+1}}{2}\sum_n (k_n-k_0)^{-p-2}(k-k_n)^{-1}\varphi_n^A(r)\,\varphi_n^A(r') \qquad (2.19)$$

($G^{+(q)}$ means q times differentiation with respect to k), where the introduction of the entire term may improve the convergence, which for $k_0 = 0,\ p \geq 1$ can be proved to be absolute and uniform, cfr. refs.[19,4] . This convergence is, though, more than needed for the Green function; only the convergence of the corresponding expression for $\int_0^a G(k,r,r')\,f(r')\,dr'$, f bounded is necessary. All the expansion of the Green function mentioned here have this convergence property.

In the classes of functions B) and C), only those with outgoing asymptotics, b) permit a direct construction of G^+, i.e., respectively

$$G_\ell^+ = \sum_n \frac{\lambda_n \varphi_n^B(n)\, \varphi_n^B(r')}{1-\lambda_n} \qquad (\lambda_n = \gamma_n^{-1}) \tag{2.20}$$

(Weinberg)

and

$$G_\ell^+ = \sum_n \frac{\varphi_n^c(r)\, \varphi_n^c(r')}{k^2 - k_n^2} \tag{2.21}$$

(Kapur-Peierls)

Note, that (21) (or (20)) is not a Mittag-Leffler expansion, the φ_n's and k_n's are k-dependent.

With the Sasakawa choice of boundary conditions, one obtains in a similar way the principal value Green function

$$G_\ell^P = \sum_n \frac{\lambda_n \varphi_n^{B,\frac{\pi}{2}}(r)\, \varphi_n^{B,\frac{\pi}{2}}(r')}{1-\lambda_n} \tag{2.22}$$

(real Weinberg $\Delta_\ell = \frac{\pi}{2}$).

A similar choice of phase could of course be made for the functions of the last line, Co), this seems though not to be in common use.

If we, instead of $\frac{\pi}{2}$ put in a general Δ_ℓ - value, we can in a similar way construct a Green function, which we can write as

$$G_\ell^\Delta = \frac{e^{i\Delta_\ell} G_\ell^+ - e^{-i\Delta_\ell} G_\ell^-}{2i \sin \Delta_\ell} \tag{2.23}$$

which, like G_ℓ^+ and G_ℓ^P , can be expanded either in terms of generalized Weinberg states, with a formula identical to (2.20) or in terms of Natural Boundary condition states, with a formula identical to (2.21).

Also the bound state Green's function $G_\ell(E<0)$ has similar expansions.

In the following, we shall consider some of the expansions in more detail, and compare different expansions with exact calculations for square well and Woods-Saxon potential.

3. The resonance functions and the Mittag-Leffler Expansion Mathematical Technique

a. The Wave Functions

The physical wave functions are solutions of the radial equation, corresponding to (2.1)

$$\frac{d^2}{dr^2}\psi_\ell + \left(k^2 - \frac{\ell(\ell+1)}{r^2} - V(r)\right)\psi_\ell = 0 \tag{3.1}$$

with the boundary conditions

$$\psi_\ell(0) = 0 \tag{3.2}$$

$$\psi_\ell(r) \underset{r\to\infty}{=} j_\ell(kr) + \frac{S_\ell - 1}{2i} h_\ell^+(kr) = \frac{i}{2}\left[h_\ell^-(kr) - S_\ell(k)\, h_\ell^+(kr)\right]$$

(Here $j_\ell, h_\ell^\pm$ are Ricati-Bessel and Ricati-Hankel functions, defined as in ref. /20/), or otherwise said, ψ_ℓ satisfies the radial Lippman-Schwinger equation

$$\psi_\ell(r) = j_\ell(kr) + \int_0^a dr' G_{o\ell}^+(k,r,r')\, V(r')\, \psi_\ell(kr) \tag{3.3}$$

$$G_{o\ell}^+(k,r,r') = -\frac{1}{k} j_\ell(kr_<)\, h_\ell^+(kr_>) \tag{3.4}$$

Going to the Born approximation limit, we see, from (3.1)-(3.4) that the function

$$\psi_\ell^G(k,r) = \frac{h_\ell^+(ka)}{k}\, \psi_\ell(k,r) \tag{3.5}$$

is bounded by

$$\psi_\ell^G(k,r) < \begin{cases} C_1\, e^{-(a-r)\beta_\ell}, & \beta_\ell > 0 \\ C_2\, |k|\, e^{(a-r)\beta_\ell}, & \beta_\ell < 0 \end{cases} \tag{3.6}$$

where $\beta_\ell = \Im m(k)$

(When $V(r)=0$ for $r > r_0$, (3.6) is obtained for $a > r_0$, see ref. /19/ for $a = r_0$). When (3.6) is fulfilled, ψ^G has Mittag-Leffler expansions

$$\psi_e^G = \sum_{i=0}^{p} \frac{k^i}{i!} \psi_e^G (0,r)^{(i)} + \sum_{n=1}^{\infty} \left(\frac{k}{k_{ne}}\right)^{p+1} \frac{C_{ne} \varphi_{ne}}{k - k_{ne}} \qquad r \leq a, \tag{3.7}$$

where

$$C_{ne} = - \frac{\varphi_{ne}(a)}{2k_{ne}} , \tag{3.8}$$

whioh for $p \geq 0$ are absolutely and uniformly oonvergent for values inside an arbitrary oontour, whioh does not oontain poles.

With Cauchy's formula, an analogue expression without an entire term, formally oorresponding to $p=-1$ in (3.7), is obtained. In some important oases, even this expression is convergent.

The asymptotio form of the φ_{ne} for $n \to \infty$ (which corresponds to complex poles) is easily seen to be

$$\varphi_{ne}(r) \approx i^{-\ell-1} \frac{e^{ik_{ne} r}}{\sqrt{2a}} , \quad r \leq a \qquad |k_{ne}| \to \infty \qquad \Im m\, k_{ne} < 0 . \tag{3.9}$$

The oomplex poles fall in pairs, so that

$$k_{\tilde{n}e} = -k_{ne}^{*} \qquad \varphi_{\tilde{n}e} = \varphi_{ne}^{*} \approx i^{e+1} \frac{e^{-ik_{ne}^{*} r}}{\sqrt{2a}} . \tag{3.10}$$

To enumerate the poles, we may arbitrarily use the system, that when we increase the well depth, starting from $\gamma = 0$, the poles whioh first meet at the imaginary axis are called 1 and 2, the next 3 and 4 and so on. Further, we can then let odd numbers denote those which move downwards on the axis, and even numbers the others (whioh beoome bound states). For the complex poles, we can let the odd numbers oorrespond to negative $Re(k)$, so that $\tilde{n} = n-1$, if n even.

For $n \to \infty$ we have

$$|Re(k_{ne})| \approx \frac{1}{a}\left(u_n - \frac{m+2}{4u_n} \ln\left[\frac{(2u_n)^{m+2}}{A^2}\right]\right) \tag{3.11}$$

$$\Im m(k_n) \approx -\frac{1}{a} \ln\left[\frac{(2u_n)^{m/2+1}}{A}\right]$$

$$u_n = n\pi - \frac{\pi}{2}\left[\frac{m}{2} + \tau\right]$$

$$\tau = \begin{Bmatrix} 0 \\ 1 \end{Bmatrix} \text{ for } (-1)^e V^{(m)}(a) \begin{Bmatrix} > 0 \\ < 0 \end{Bmatrix}$$

Here $V^{(m)}(a) \neq 0$, $V^{(n)}(a)$ $(n < m) = 0$ (but we oan, without loss of generality assume $m = 0$, chosing $a = r_0 + d$, d arbitrarily small).

We see from this, that(3.7) is oonverging as n^{-2} for $p = m+1$, and, for $p > m+1$ $n^{-2-(p-m-1)}$, so the convergence of the Mittag-Leffler expansion is easily promoted, by ohosing a suffioiently large p .

b. The S-matrix

It was shown in /4/, that the expression

$$F_e(k) \equiv \left(\frac{S_e(k)-1}{2ik}\right)\left(h_e^{+}(ka)\right)^2 \tag{3.12}$$

and therefore also the S-matrix has absolutely and uniformly convergent Mittag-Leffler expansions for $p \geq m+1$ (see above)

$$S_e(k) = 1 + 2ik\left(h_e^{+}(ka)\right)^{-2}\left(\sum_{q=0}^{p} \frac{k^q}{q!} F^{(q)}(0) + \sum_{n=0}^{\infty} \left(\frac{k}{k_{ne}}\right)^{p+1} \frac{C_{ne}\varphi_{ne}(a)}{k - k_{ne}}\right) \tag{3.13}$$

On the other hand, the Mittag-Leffler (or Cauohy) expansion for the Green function (2.18) with no entire term $(p=-1)$ is also convergent, in an operator sense, operating inside $r=a$.

Since the S-matrix can be determined from integrals of the wave function or the Green function, it should be expected, that with a given p , suoh formulae oan be used to obtain more rapidly converging expressions for the S-matrix.

Actually we have /20/

$$S_e(k) = 1 - \frac{2i}{k} \int_0^a dr\, j_e(kr)\, V(r)\, \psi_e(k,r) \tag{3.14}$$

from which, by means of (3.7), we obtain

$$S_e(\kappa) = 1 - 2i[h_e^+(\kappa a)]^{-1}\left(\sum_{i=0}^{p} \frac{\kappa^i}{i!} \langle j_e|V|e_i\rangle + \sum_n \left(\frac{\kappa}{\kappa_{ne}}\right)^{p+1} \frac{c_{ne}\langle j_e|V|\varphi_{ne}\rangle}{\kappa-\kappa_{ne}}\right), \tag{3.15}$$

where

$$\langle j_e|V|e_i\rangle \equiv \int_0^a j_e(\kappa r)V(r)\psi_e^{(i)}(0,r)\,dr \tag{3.16a}$$

$$\langle j_e|V|\varphi_{ne}\rangle \equiv \int_0^a j_e(\kappa r)V(r)\varphi_{ne}(r)\,dr \tag{3.16b}$$

In terms of the Green function, S is expressed by

$$S_e(\kappa) = 1 - \frac{2i}{\kappa}\left\{\int_0^a dr\, j_e(\kappa r)V(r)j_e(\kappa r) + \int_0^a dr\int_0^a dr'\, j_e(\kappa r)V(r)G_e^+(\kappa,r,r')V(r')j_e(\kappa r')\right\} \tag{3.17}$$

Introducing here (2.19) ($\kappa_0 = 0$), we get

$$S_e(\kappa) = 1 - \frac{2i}{\kappa}\left\{\sum_{i=0}^{p}\frac{\kappa^i}{i!}\int_0^a dr\int_0^a dr'\, j_e(\kappa r)V(r) G_e(0,r,r')^{(i)}V(r')j_e(\kappa r') + \sum_n\left(\frac{\kappa}{\kappa_{ne}}\right)^{p+1}\frac{\langle j_e(\kappa)|V|\varphi_{ne}\rangle^2}{2\kappa_{ne}(\kappa-\kappa_{ne})} + \langle j_e(\kappa)|V|j_e(\kappa)\rangle\right\} \tag{3.18}$$

which is identical to the formula of ref. [21] if we chose p=-1.

At the threshold we have [10]

$$S_e(\kappa) - 1 = O(\kappa^{2e+1}) \quad \kappa\to 0\,. \tag{3.19}$$

In this sense, all the three expansions, (3.13), (3.15) and (3.18) show the correct threshold behaviour, independent of the number of terms in the expansion, since

$$\kappa[h_e^+(\kappa a)]^{-2} = O(\kappa^{2e+1}) \quad \kappa\to 0 \tag{3.20}$$

$$[h_e^+(\kappa a)]^{-1}\langle j_e(\kappa a)|V|e_i\rangle = O(\kappa^{2e+1}) \quad \kappa\to 0$$

$$\frac{1}{\kappa}\langle j_e(\kappa)|V|j_e(\kappa)\rangle = O(\kappa^{2e+1}) \quad \kappa\to 0 \tag{3.21}$$

$$\frac{1}{\kappa}\int_0^a dr\int_0^a dr'\, j_e(\kappa r)V(r)G_e(0,r,r')V(r')j_e(\kappa r') = O(\kappa^{2e+1}) \quad \kappa\to 0$$

For $\kappa\to\infty$, we must have $S(\kappa)\to 1$, and the expressions (3.15) and (3.18) do actually fulfil this requirement, since for large k-values, the $j_e(\kappa r)$ are rapidly oscillating, so the integrals tend to zero. Since the expansion (3.13) is uniformly convergent, it must also give the correct asymptotic behaviour, but in this case only after summation over a large number of terms.

In general, the above argument leads us to expect, that the expression (3.15) converges faster than (3.13) and (3.18) faster than (3.15). In analogy with what was just said about amelioration of the convergence of the Mittag-Leffler expansions for S, faster converging expressions for the continuum wave function can also be obtained, using integral equations.

From [10]

$$\psi_e(\kappa,r) = j_e(\kappa r) + \int_0^a G_e(\kappa,r,r')V(r')j_e(\kappa r')\,dr' \tag{3.22}$$

and the expansion (2.19), we obtain

$$\psi_e(\kappa,r) = j_e(\kappa r) + \sum_{i=0}^{p}\frac{\kappa^i}{i!}\int_0^a G_e(0,r,r')^{(i)} V(r')j_e(\kappa r')\,dr' + \sum_{n=1}^{\infty}\left(\frac{\kappa}{\kappa_{ne}}\right)^{p+1}\frac{\varphi_{ne}(r)\langle j_e(\kappa)|V|\varphi_{ne}\rangle}{2\kappa_{ne}(\kappa-\kappa_{ne})}\,. \tag{3.23}$$

Conclusion

We have here considered different discrete expansions of continuum wave functions. The different sets have in common, that they are complete in a finite region $r \leq a$ that the functions in the set satisfy Schrödinger-like equations, and that at the boundary $r = a$, they satisfy such conditions, that they can be joint with a solution of the free particle Schrödinger equation for $r > a$.

The usefulness of such expansions depend on orthogonality relations and other equations, used to determine expansion coefficients, and on the fastness of the convergence of the expansion. For the problems, in which these sets are used, the expansions of Green functions are particularly important. We have here discussed these aspects of the different expansions. The convergence problems will be treated and illustrated with numerical examples in a later publication, which will also contain a more detailed discussion of the new type of real Weinberg functions, introduced here.

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