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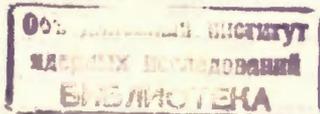**J.Bang, F.A.Gareev, M.H.Gizzatkulov,**

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EXPANSION OF CONTINUUM FUNCTIONS ON RESONANCE WAVE FUNCTIONS AND AMPLITUDES. I.

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EXPANSION OF CONTINUUM FUNCTIONS ON RESONANCE WAVE FUNCTIONS AND AMPLITUDES. I.

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Банг Е. и др.   E4 - 11377

   Разложение функций континуума по резонансным волновым
   функциям и амплитудам. I.

   Строго математически рассмотрено полюсное разложение (согласно
теореме Миттаг-Леффлера) волновых функций, амплитуд рассеяния и
функций Грина при положительных энергиях. Получен и обсуждается общий
вид этих разложений для конечных потенциалов, а также для кулоновско-
го потенциала. Показана возможность применения данного метода в ядер-
ных структурных расчетах.

   Работа выполнена в Лаборатории теоретической физики, ОИЯИ.

Bang J. et al.   E4 - 11377

   Expansion of Continuum Functions on Resonance Wave
   Functions and Amplitudes. I.

   The pole expansion (Mittag-Leffler expansion) of wave functi-
ons, scattering amplitudes and Green's functions at positive energi-
es are discussed in a mathematically rigorous way. The general
proofs of convergence are supplemented by numerical calculations
which, for simple examples, show the convergence to be fast. Ap-
plications of the method to nuclear structure calculations are discus-
sed.

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

1. Introduction

   In nuclear physics, the problem of treating states with
positive energy on an equal footing with bound states, has for
a long time drawn the attention of several authors[1]. Here we
are specially thinking of the single particle states used as
basis in, e.g., shell model calculations or more approximate
many body descriptions of nuclear structure. In such calculations,
the continuum states must be included in order to have a complete
expansion basis. The necessity of this has recently become more
urgent, due to the growing interest in studying the giant reso-
nances and other highly excited states, where the continuum ad-
mixtures are particularly important. Apart from the more con-
ventional problem of single particle scattering, these states
also play a direct role as final states or intermediate states
in many nuclear reactions, like (d,p) processes, etc.

   The fact that the spectrum of positive energy states is con-
tinuous, and the states not square integrable, gives rise to a
number of problems when these states are used as basis states in
realistic calculations of the above-mentioned type. Therefore,

in such calculations, the single particle potential is often approximated by one, which has only a discrete spectrum, like the harmonic oscillator or the infinite square well, but the unphysical character of these potentials leads to complications connected with bad convergence of the expansion in certain regions of space. In general we can say that if a physical problem is solved by the method of expansion in a complete set, the convergence will be best if the basis functions, or at least some of them, are similar to the physical function, i.e., if they are solutions of an equation of a similar type, with similar boundary conditions.

A number of ways have been proposed to construct discrete sets of wave functions, which give uniform convergence of the expansion when certain conditions are fulfilled. The bases of Eisenbud and Wigner[2], however, share the property of unphysical boundary conditions with those mentioned above. The basis functions of Kapur and Peierls[3] and the Weinberg[4,5] functions form complete sets for positive energies, and the Sturm-Liouville functions give absolute and uniform (or stronger than uniform) convergence for expansion of square integrable functions[6,7].

In contrast to the bound states these discrete sets present the inconvenience that they are energy-dependent. In reaction calculations, this may lead to some advantages, but in the solution of a physical problem by expansion in a complete set, it is desirable that only the expansion coefficients contain the energy dependence.

A natural generalization of the discrete bound state solutions of the Schrödinger equation to positive (or rather complex) energy values was introduced by Gamow in the description of α-decay[8]. Like the bound states, these states have energies which correspond to poles of the S-matrix. A representation of the S-matrix by means of its poles was given by Peierls[9]. A theory of nuclear reactions, in which these poles are used for expansion of the reaction amplitudes, was developed by Humblet and Rosenfeld[10].

Since the Gamov functions (which in the following we shall call the resonance functions) are increasing exponentially with r, the usual definitions of normalization, orthogonality and completeness are not valid for these functions. This is, to our mind, the main reason why they have not become more widely used.

Lately, a number of methods of normalization of the resonance wave functions were suggested, all of which, however, are equivalent to the method of Zel'dovich[11-15] (but for the antibound states some of these methods are not valid).

Recently, techniques for expansion of continuum wave functions over resonance functions were developed, using the analytic properties of Green's functions. But in this approach it is in general difficult to answer the question of convergence of this expansion.

It is in this connection an important observation that in the study of the analytic properties of the S-matrix, and of its expansion in pole terms, the theorem of Mittag-Leffler[16] played a decisive role, guarantying that the series converges uniformly inside an arbitrary closed contour, which contains no poles. It is therefore tempting to use this theorem also for the expansion of the wave functions of the continuous spectrum, and of the Green's functions.

We are here using the expressions obtained in this way for comparison with exact solutions in some concrete cases, following the work of Serdobolskij[17]. In some of the works, where Gamow states are introduced, they are used in matrix elements, say, for calculation of transition amplitudes or expansion coefficients, involving integrations over all space. The exponential growth with r of these states is then neutralized by introduction of a regularization factor. Although in some cases, as,e.g.,with the normalization integral[11] this procedure is unambiguous, we shall here stick to the more conservative idea of using the resonant states as a basis for calculation of such matrix elements, where we need only the properties of the wave functions inside a finite radius, R. We, therefore, also, like many of the above-mentioned authors, only need to prove the expansion theorems we are going to use for this finite region.

II. The Mittag-Leffler expansion

a) The Mittag-Leffler expansion (MLE) of the S-matrix

We shall here, and in the following, assume that our single particle potential $V(r)$ is spherical, identically zero for $r > R$, and has no singularities (except for a numerical example, where a δ-function potential is used). These conditions are stronger than necessary to prove the theorems used in the following, but reasonable from the point of view that we are concerned with nuclear problems. The Coulomb potential, as met in atomic and molecular physics is hereby excluded, but the repulsive Coulomb force important for protons and α-particles is treated below.

With the above restrictions, the Jost functions $f_\ell(k)$ are holomorphic in the whole k-plane. We shall further assume that they have only simple zeroes in the k-plane. In the Appendix we throw some light on this assumption. For $S_\ell(k) = f_\ell(k)/f_\ell(+k)$, we can now prove that the function

$$F_\ell(k) \equiv \frac{S_\ell(k) - 1}{2ik}\left(h_\ell^+(kR)\right)^2 \tag{2.1}$$

for a large closed contour in the k-plane, i.e. $|k| > |k_c|$, which does not come near to any pole, - it can be proved that such contours do exist, - we will have

$$F_R < \text{constant} \cdot |k_c|^{P_0},$$

where P_0 is a non-negative integer. For a potential, of which the mth derivative at $r = R$ is different from 0, it can be proved that $P_0 \leq m + 2$.

Let us denote the poles of F_R by k_n, and the corresponding residue by r_n. The MLE theorem then states that if the poles are ordered according to increasing (or non-decreasing) value of $|k_n|$, the expansion

$$F_\ell(k) = \sum_{q=0}^{p} \frac{k^q}{q!} F_\ell^{(q)}(o) + \sum_{n=1}^{\infty}\left(\frac{k}{k_n}\right)^{p+1}\frac{r_n}{k - k_n} \tag{2.2}$$
$$p \geqslant p_0$$

converges uniformly in the k-plane within any closed contour which does not contain poles. So, expressing S by (2.1)

$$S_\ell(k) = 1 + 2ik\left(h_\ell^+(kR)\right)^{-1}\cdot F_R(k) \tag{2.3}$$

we have the different MLE of S. A MLE contains in general an entire function and a series of pole terms. This division is however not unique, it can be changed by a re-ordering of the expansion, as exemplified by the choice of p above. The conditions $p \geqslant p_0 > 0$ are sufficient conditions, but not necessary; in the example of a δ-potential, given below, p = -1 gives a convergent series.

The advantage of the presentation of the MLE given above is, that the entire function is given, for any value of p. The pole series itself will, of course, converge faster for lage p-values, as we shall see in some concrete examples below. It should be noted, that since $S_\ell(k) - 1 \underset{k \to 0}{=} O(k^{2\ell+1})$ (except for the case of a bound state at zero energy), that in general $F_R(o) \neq 0$ since $h_\ell^+(kR) = O(k^{-\ell})$ for $k \to 0$.

b) The MLE of the wave function

In order to apply the expansion of the S-matrix obtained above, in the most direct way to the scattering states, let us introduce the function

$$\Psi_\ell^G \equiv \frac{e^{-\frac{1}{2}i\pi\ell}}{k} h_\ell^+(kR)\,\Psi_\ell^{(+)}(z). \tag{2.4}$$

So Ψ_ℓ^G satisfies the radial Schrödinger equation and for all $z \leqslant R$, we have

$$\frac{d^2}{dz^2}\Psi_\ell^G + \left(k^2 - \frac{\ell(\ell+1)}{z^2} - V(z)\right)\Psi_\ell^G = O \tag{2.5}$$

and for all $z \geqslant R$, we have

$$\Psi_\ell^G = \frac{h_\ell^+(kR)\,e^{-\frac{i}{2}\pi\ell}}{k}\left(j_\ell(kz) + \frac{S_\ell(k) - 1}{2i}h_\ell^+(kz)\right), \tag{2.6}$$

where j_ℓ and h_ℓ^+ are Riccatti-Bessel and Ricatti-Hankel functions of the first sort, defined as in ref. /18/.

The regular solution of the radial Schrödinger equation occurs in the literature under different names, corresponding to different k-dependent normalizations. Our reason to introduce one more variant, our Ψ_ℓ^G, will become clear in the following.

Now, at the poles k_n of the S-matrix, also the wave function has poles. Its residues must be wave functions, which satisfy

the same Schrödinger equation as Ψ_ℓ^G (or $\Psi^{(+)}$), for $\kappa = \kappa_n$ but for $\tau > R$ become proportional to h_ℓ^+ , so

$$\lim_{\kappa \to \kappa_n} (\kappa - \kappa_n)\, \Psi_\ell^G(\kappa, \tau) = c_n\, \varphi_n(\tau) \qquad (2.7)$$

where the $\varphi_n(\kappa_n, \tau)$ are solutions of the eigenvalue problem

$$\frac{d^2}{d\tau^2} \varphi_n(\tau) + (\kappa_n^2 - \frac{\ell(\ell+1)}{\tau^2} - V(\tau))\, \varphi_n(\tau) = 0 \qquad (2.8)$$

$$\varphi_n(0) = 0 \qquad (2.8a)$$

$$h_\ell^+(\kappa_n R)\, \frac{d}{d\tau} \varphi_n(\tau)\Big|_{\tau=R} = \varphi_n(R)\, \kappa_n\, h_\ell^{+\prime}(\kappa_n R). \qquad (2.8b)$$

The constant c_n must depend on the normalization of the φ's . These functions are identical to the bound states for $\mathrm{Re}(k_n)=0$, $\mathrm{Im}(k_n) > 0$. For $\mathrm{Re}(\kappa_n) = 0$, $\mathrm{Im}(\kappa_n) < 0$ they are antibound states and for complex κ_n values resonant states, among these the Gamow states for $\mathrm{Re}(\kappa_n) > 0$.

The normalization of these functions is naturally some generalization of the normalization prescription for bound states. Keeping in mind, that we only want to use the properties of the wave functions for $\tau \leqslant R$, we shall use the normalization

$$\int_0^R d\tau\, \varphi_n^2(\tau) + \frac{\varphi_n^2(R)}{2\kappa_n}\left[\frac{d}{d\kappa}\left(\frac{\kappa\, h_\ell^{+\prime}(\kappa R)}{h_\ell^+(\kappa R)}\right)\right]_{\kappa=\kappa_n} = 1. \qquad (2.9)$$

This has, e.g., the advantage of giving the same 1. order expression for resonance energy changes in the continuum as in bound states.

Now, the constant c_n is determined to be

$$c_n = -\frac{e^{-\frac{i}{2}\pi\ell}}{2\kappa_n}\, \varphi_n(R) \qquad (2.10)$$

A detailed derivation of c_n for the case $\ell = 0$ is given below. Once the residues are given, the MLE of the function Ψ_ℓ^G can be constructed

$$\Psi_\ell^G(\kappa, \tau) = \sum_{i=0}^{P} \frac{\kappa^i}{i!}\, \Psi_\ell^G(0, \tau)^{(i)} + \sum_{n=1}^{\infty} \left(\frac{\kappa}{\kappa_n}\right)^{P+1} \frac{c_n\, \varphi_n(\tau)}{\kappa - \kappa_n} \qquad (2.11)$$

for $p = \ell = 0$, this series coincides, apart from the normalization, with the formula of ref.[17].

That the Ψ_ℓ^G can be represented by a MLE is most easily shown by considering the relation between Ψ_ℓ^G and the Green function

$$G^+ = -\kappa^{-1}\, \Psi_\ell^+(\kappa, \tau_<)\, f_\ell(\kappa, \tau_>)\, e^{-\frac{i\pi\ell}{2}} \qquad (f_\ell(\kappa, \tau > R) = h_\ell^+(\kappa\tau))$$

$$\Psi_\ell^{-G}(\kappa, \tau) = -G^+(\kappa, \tau, R) \qquad (2.12)$$

So, the expansion properties of Ψ_ℓ^G are given by those of G^+, which we shall study in the next section.

It should be noted, that the advantage of presenting the scattering wave function as a sum of energy-independent functions, multiplied with energy-dependent coefficients is shared by all the MLE with different p. The choice of p is to a large degree a matter of convenience, since already for $p = -1$, the expansion will often be convergent , but it means, that the convergence can be improved, at the cost of enlarging the number of functions $\Psi_\ell^G(0, \tau)$

These are found as solutions with the proper boundary conditions of differential equations, derived from the Schrödinger equation. The equations for $i = 0$ and $i = 1$ are, e.g., both

$$\frac{d^2}{d\tau^2} \Psi_\ell^G(0, \tau)^{(i)} - \left(\frac{\ell(\ell+1)}{\tau^2} + V(\tau)\right) \Psi_\ell^G(0, \tau)^{(i)} = 0 \qquad (2.13)$$

and the boundary conditions

$$\Psi_\ell^G(0, 0)^{(0)} = \Psi_\ell^G(0, 0)^{(1)} = 0 \qquad (2.13a)$$

$$e^{\frac{i\pi\ell}{2}} \Psi_\ell^G(0, R)^{(0)} = F_R(0) + \frac{R}{2\ell+1} \qquad (2.13b)$$

$$e^{\frac{i\pi\ell}{2}} \Psi_\ell^G(0, R)^{(1)} = R F_R^{-1\prime}(0) + iR^2 \delta_{\ell 0} \qquad (2.13c)$$

C. The MLE of the Green function. Completeness relation

The MLE of the Green function was considered by several authors[13,23].

The simplest way to obtain such an expansion is presumably to start with the general expression for the radial equation Green function G^+

$$G_\ell^+(\kappa, \tau, \tau') = \sum_{n(\text{bound})} \frac{\varphi_n(\tau)\, \varphi_n(\tau')}{\kappa^2 - \kappa_n^2} + \frac{1}{\pi}\int_{-\infty}^{+\infty} \frac{d\kappa'}{\kappa'} \frac{\Psi_\ell^+(\kappa', \tau)\, \Psi_\ell^{+*}(\kappa', \tau')}{\kappa^+ - \kappa'} \qquad (2.14)$$

$$(\kappa^+ = \kappa + i\gamma, \gamma \to 0).$$

The integral may be calculated, using theorem, by closing the contour in the lower half plane for such terms where that integral becomes small and in the upper half plane (counter clockwise) for the other terms, each time using a large contour, that does not come near to any pole. That such contours exist, was already mentioned above.

Now the contributions from the poles with positive imaginary k-value will partly cancel the bound state part of G_ℓ^+ and the contribution from $K^+ (\gamma \to 0+)$ vanishes, leaving us with

$$G_\ell^+(K,\tau,\tau') = \sideset{}{'}\sum_{n\,(all\,poles)} \frac{\varphi_n(\tau)\,\varphi_n(\tau')}{2\,K_n(K-K_n)}$$

(2.15)

$$(\tau,\tau' < R)$$

where the $\varphi_n(\tau)$ are the resonance functions, with the same normalization which was introduced earlier. We see that the Green function, for the case considered, has a MLE with p=-1. The same must therefore be the case for $\Psi_\ell^+ (\tau \le R)$.

Furthermore, as was pointed out by Romo, the Green function for $K \to \infty$ must behave as $\frac{\delta(\tau-\tau')}{K^2} + O(K^{-3})$. From this one concludes

$$\frac{1}{2}\sideset{}{'}\sum_{n} \varphi_n(\tau)\,\varphi_n(\tau') = \delta(\tau-\tau')$$

(2.16)

$$(\tau,\tau' < R)$$

and

$$\sum_n \varphi_n(\tau)\,\varphi_n(\tau')/K_n = 0 .$$

(2.17)

The first equation can be stated as an overcompleteness relation. Note, that the presence of the factor 1/2 is not merely a question of normalization, since it appears with the bound states also, where, for large values of R, this plays no role. The second relation of course also indicates very high degree of linear dependence among the φ_n's.

The fact, that we have completeness only within a limited volume, may seem a drawback, but it is related to the large difficulties encountered, if one wants to use the Ψ's as expansion basis in all space. The regularization method tries to overcome these difficulties, but if the inner product of two state vectors is defined with that method, the linear dependence (2.17) is conserved , but the completeness is lost, even at the point where it is most needed, as seen from the following example, with

ℓ =0. For $\tau > R$

$$\Psi^G(\kappa,\tau) = \frac{e^{R i \kappa}}{2i k}(S(\kappa)e^{ik\tau} - e^{-ik\tau})$$

(2.18)

$$\varphi_n(\tau) = \varphi_n(R)\,e^{iK_n(\tau-R)} .$$

(2.19)

So for the regularized overlap integral between Ψ^G and φ_n we get

$$\lim_{\varepsilon \to 0}\int_0^\infty \Psi^G(\tau)\,\varphi_n(\tau)\,e^{-\varepsilon\tau^2}\,d\tau =$$

$$=\int_0^R \Psi^G(\tau)\,\varphi_n(\tau)\,d\tau + \varphi_n(R)\frac{e^{i(k-K_n)R}}{2ik}\int_R^\infty (S(\kappa)e^{i(K_n+\kappa)\tau} - e^{i(K_n-\kappa)\tau})\,d\tau =$$

$$=\int_0^R \Psi^G(\tau)\,\varphi_n(\tau)\,d\tau - \varphi_n(R)\frac{e^{i(k-K_n)R}}{2ik}\left[\frac{S(\kappa)e^{i(K_n+\kappa)R}}{i(K_n+\kappa)} - \frac{e^{i(K_n-\kappa)R}}{i(K_n-\kappa)}\right] =$$

(2.20)

$$=\int_0^R \Psi^G(\tau)\,\varphi_n(\tau)\,d\tau + \varphi_n(R)\left[\frac{i}{K_n+\kappa}\frac{S(\kappa)e^{2ikR}-1}{2ik} + \frac{1}{2\kappa(K_n+\kappa)} - \frac{1}{2\kappa(K_n-\kappa)}\right] =$$

$$=\int_0^R \Psi^G(\tau)\,\varphi_n(\tau)\,d\tau + \varphi_n(R)\left[\frac{i}{K_n+\kappa}\Psi^G(R) - \frac{1}{K_n^2 - K^2}\right]$$

but this is zero, acccording to (2.28) below.

The expression for the Green function, given above, may also, using (2.17), be written in a number of other ways, which may be useful in different contexts

$$G^+ = \frac{1}{2}\sum_n \frac{\varphi_n(\tau)\varphi_n(\tau')}{K^2 - K_n^2} + \frac{1}{2}\sum_n \frac{K}{K_n}\frac{\varphi_n(\tau)\varphi_n(\tau')}{K^2 - K_n^2} .$$

(2.21)

Here, the first term, which is even in K, represents the real part of the Green function, whereas the second , odd, term represents the imaginary part of G^+ (for real K). Another interesting formula is

$$G^+ = \sum_n \frac{\varphi_n(\tau)\varphi_n(\tau')}{K^2 - K_n^2} + \frac{1}{2}\sum_n \frac{1}{K_n}\frac{\varphi_n(\tau)\varphi_n(\tau')}{K + K_n} .$$

(2.22)

Here, the first term contains the poles, whereas the second term is regular at the points $K = K_n$. For a sufficiently narrow resonance, i.e.,if $K_n = \mathscr{x}_n + i\gamma_n$, that $|\gamma_n|$ is sufficiently small, the pole term gives the usual resonance expression for Ψ^+

$$\Psi^+ \infty \frac{\varphi_n(\tau)\,\varphi_n(R)}{K^2 - (\mathscr{x}_n^2 - \gamma_n^2 - 2i\mathscr{x}_n\gamma_n)} .$$

(2.23)

d. The relations between $\Psi^G(\kappa,z)$ and $\varphi_n(z)$ normalization

In this section, we shall for simplicity consider the case of $\ell = 0$ only.

We shall, for this case, derive some usefull relations between Ψ^G and φ_n .

For $\ell = 0$, we have, for $z > R$

$$\Psi^G(\kappa,z) = e^{i\kappa R}\left(\frac{\sin\kappa z}{\kappa} + \frac{S(\kappa)-1}{2i\kappa}\, e^{i\kappa z}\right) \tag{2.24}$$

$$\frac{d}{dz}\Psi^G(\kappa,z)\Big/_{z=R} = i\kappa\, \Psi^G(\kappa,z) + 1 \tag{2.24a}$$

$$\varphi_n(z) = \varphi_n(R)\, e^{i\kappa_n(z-R)} \tag{2.25}$$

$$\Psi^G(\kappa,0) = \varphi_n(0) = 0 \tag{2.25a}$$

Further

Now Ψ^G and φ_n satisfy, respectively, the Schrödinger equations

$$\frac{d^2}{dz^2}\Psi^G + (\kappa^2 - V)\Psi^G = 0 \tag{2.26}$$

and

$$\frac{d^2}{dz^2}\varphi_n + (\kappa_n^2 - V)\varphi_n = 0 . \tag{2.27}$$

Multiplying the first equation by φ_n and the second by Ψ^G , subtracting and integrating from 0 to R, we get

$$-(\kappa^2 - \kappa_n^2)\int_0^R \Psi^G \varphi_n\, dz + i(\kappa_n - \kappa)\Psi^G(R)\varphi_n(R) = \varphi_n(R) \tag{2.28}$$

now

$$c_n\varphi_n(z) = \operatorname*{res}_n\left(\Psi^G(\kappa,z)\right) = \lim_{\kappa \to \kappa_n}\left((\kappa-\kappa_n)\Psi^G(\kappa,z)\right) \tag{2.29}$$

so

$$2\kappa_n c_n\int_0^R \varphi_n^2\, dz + i c_n \varphi_n^2(R) = -\varphi_n(R) \tag{2.30}$$

or, since

$$c_n = -\frac{\varphi_n(R)}{2\kappa_n} \tag{2.31}$$

$$\int_0^R \varphi_n^2(z)\, dz + i\frac{\varphi_n^2(R)}{2\kappa_n} = 1 \tag{2.32}$$

If instead, we take another residuum, $\operatorname*{res}_m\left(\Psi^G(\kappa,z)\right)$ we obtain

$$\int_0^R \varphi_n(z)\varphi_m(z)\, dz + i\frac{\varphi_n(R)\varphi_m(R)}{\kappa_n + \kappa_m} = \delta_{nm} . \tag{2.33}$$

e. Charged particles

In the case of charged particles, the solutions for $z \to \infty$ do not have the same simple form as for neutrons. We shall still assume that the nuclear potential is 0 for $r > R$.

In the place of the Riccati-Hankel function, we must then introduce the Whittaker functions, W , so that (2.6) is replaced by

$$\Psi_\ell^{G(\kappa)} = \frac{e^{-\frac{i}{2}\pi\ell}}{2i\kappa} W_{-i\eta,\ell+\frac{1}{2}}(-2i\kappa R)\times$$
$$\times\left(S_\ell^{(\kappa)}(\kappa)W_{i\eta,\ell+\frac{1}{2}}(-2i\kappa z) - W_{i\eta,\ell+\frac{1}{2}}(2i\kappa z)\right) . \tag{2.34}$$

Here,

$$\eta = \frac{Z_1 Z_2 e^2 \mu}{\kappa} , \tag{2.35}$$

where $Z_1 e$, $Z_2 e$ are the charges of the projectile and the fixed scatterer and μ their reduced mass.

The solutions of the radial equation which continue $W_{-i\eta}$ and $W_{i\eta}$ do then correspond to the usual f_+ and f_- , respectively. The natural generalization of the usual way of finding the singularities of $S_\ell(\kappa)$, is to look at the integral equation, satisfied by f_-

$$f_-(\kappa,z) = f_-^{(o)}(\kappa,z) + \int_z^R d\rho\, B(\ell,\kappa,z,\rho)V(\rho)f_-(\kappa,\rho) , \tag{2.36}$$

where the Green function B is given by

$$B(\ell,\kappa,z,\rho) = \frac{1}{2i\kappa}\left(f_-^{(o)}(\kappa,z)f_+^{(o)}(\kappa,\rho) - f_+^{(o)}(\kappa,z)f_-^{(o)}(\kappa,\rho)\right) . \tag{2.37}$$

We are free in choosing $V(\rho)$ and $f^{(o)}$. Since the singularity at r=0 of the point charge Coulomb potential does not occur for realistic charge distributions, the simplest choice is perhaps to say, that V is the total potential, nuclear and electrostatic, inside R, and that $f_\pm^{(o)}$ therefore are the combination of the Riccati-Hankel functions, e.g.

$$f_-^{(o)} = a_-(\kappa)h^- + a_+(\kappa)h^+ . \quad (z \leq R) . \tag{2.38}$$

Note, that in spite of our boundary conditions being different

from those of de Alfaro and Regge[19], B is identical to the one of ref.[19].

It is therefore estimated , e.g., by

$$|B| < C^{|b|\varsigma + b\imath} \left(\frac{\varsigma}{1+|\kappa|\varsigma}\right)^{\ell + \frac{1}{2}} \left(\frac{\imath}{1+|\kappa|\imath}\right)^{-\ell + \frac{1}{2}} \qquad (2.39)$$
$$(\ell = Im(\kappa)) .$$

From (2.36) and (2.38) we must also have

$$f_-(\imath) = a_- f_{--}(\imath) + a_+ f_{-+}(\imath) , \qquad (2.40)$$

where $f_{--}(R) = h^-(R)$, etc.,so that we can solve the Volterra equation (2.36) for f_{--} and f_{-+} separately

$$f_{-\pm}(\imath) = h^\pm(\imath) + \int_\imath^R d\varsigma \, B(\varsigma) V(\varsigma) f_{-\pm}(\varsigma) . \qquad (2.41)$$

From this we find, using a restricted V and repeating the argumentation of ref.[16] or [19] that $f_{-\pm}$ have no other singularities than the behaviour as $(\kappa\imath)^{-\ell}$ for $\kappa\imath \to O$. The problem of the analytic structure is then reduced to finding $a_\pm(\kappa)$, i.e., to the well known determination of the proton transmission coefficient[20]. In this problem the centrifugal barrier is of minor importance, and we shall only look at $\ell = O$. So we have

$$a_+ e^{i\kappa R} + a_- e^{-i\kappa R} = W_{-i\eta, \frac{1}{2}}(-2i\kappa R)$$
$$i\kappa(a_+ e^{i\kappa R} - a_- e^{-i\kappa R}) = -2i\kappa W'_{-i\eta, \frac{1}{2}}(-2i\kappa R) \qquad (2.42)$$

or, introducing $\quad \varsigma = -i\kappa R$

$$W = e^{-\varsigma} 2\varsigma \, \Psi(1+i\eta, 2, 2\varsigma)$$
$$W' = (-1 + \frac{1}{\varsigma} + 2\frac{\Psi'}{\Psi})W \qquad (2.43)$$

$$a_\pm = \frac{1}{2} e^{\mp\varsigma} (W \mp 2 W')$$
$$\qquad (2.44)$$

$$\frac{\Psi'}{\Psi} = 1 - \frac{\Psi(1+i\eta, 3, 2\varsigma)}{\Psi(1+i\eta, 2, 2\varsigma)}$$

$$\lim_{\varsigma \to O} \frac{\Psi'}{\Psi} = 1 - \frac{(2\varsigma)^{-2} \Gamma(2)/\Gamma(\alpha) + O(\log(\varsigma))}{(2\varsigma)^{-1} \Gamma(1)/\Gamma(\alpha) + O(1)} \qquad (2.45)$$

$$= 1 - (2\varsigma)^{-1} + O(\varsigma \log(\varsigma)) \qquad (\alpha = 1 + i\eta)$$

so $W' = W(1 + O(\varsigma \log(\varsigma)))$ $(\varsigma \to O)$. So, the a's have no other singular point than k=0, where W has an essential singularity,

since it behaves as

$$W \infty (\Gamma(1-i\eta))^{-1} \qquad (2.46)$$

(or in the general case as $(\Gamma(\ell+1-i\eta))^{-1}$). So, the Jost function

$$f(\kappa) = f_-(\kappa, 0) \qquad (2.47)$$

will contain this factor

$$f(\kappa) = f^V(\kappa) / \Gamma(\ell+1-i\eta) \qquad (2.48)$$

but $f^V(\kappa)$ is holomorphic.

Consequently, also S can be written as

$$S^V = S^c \frac{\Gamma(\ell+1-i\eta)}{\Gamma(\ell+1+i\eta)} , \qquad (2.49)$$

where S^V is meromorphic. Equation (2.49) is the general expression for S with a potential which contains both Coulomb and finite range parts.

Both terms in $\Psi_\ell^{G(c)}$ will contain the factor $|\Gamma(\ell+1+i\eta)|^{-2}$, but

$$\Psi_\ell^{G(V)} = |\Gamma(\ell+1+i\eta)|^2 \Psi_\ell^{G(c)} \qquad (2.50)$$

is obviously meromorphic, as also the similar expression for the Green function. For those expressions, we can then construct different MLE , with convergence properties practicaly identical to those of the proceeding section.

III. Structure problems

The resonance functions may be a convenient tool for calculation of cross sections,e.g.,of particle transfer.

Another, and perhaps more important application is to nuclear structure calculations for such cases, where continuum admixtures play an essential role. Such calculations are often conveniently performed in other discrete basis sets, like the Sturmian or oscillator functions. However, when the total energy of the system is above some particle emission threshold these bases are seriously insufficient.

We shall therefore here study the use of the resonance functions in nuclear structure problem, looking at two cases, which are each representative of a large class of such problems.

In both cases, we shall stick to the simplest possible model of at most one particle being in a continuum state.

In this system, in principle, all energy values above a threshold energy are eigenvalues, and we shall in the first case only be concerned with finding the wave function. Let us for simplicity assume, that the other degrees of freedom are represented by one particle, which is different from the one with the threshold, so that no antisymmetrization effects occur, and that when the one particle is in the continuum, only one state of the other is, for energetical reasons, important. Futher, we shall assume zero angular momentum. So, using the Feshbach projection formalism, we write our wave function

$$\Psi = Q\Psi + P\Psi \qquad (3.1)$$

where, in this simple case

$$P\Psi = \varphi_{20}(z_2) \int_0^\infty d\kappa\, c(\kappa)\, \Psi^+(\kappa, z_1) \qquad (3.2)$$

$$Q\Psi = \sum_n c_n \varphi_n(z_1, z_2). \qquad (3.3)$$

We shall further assume $H_{PP}\,(=PHP)$ and $H_{QQ}\,(=QHQ)$ to be diagonal. The first means, that the $\Psi^+(\kappa)$ are optical model wave functions, with the important part of the residual interaction

$$\langle \varphi_{20}(z_2) \mid V_{res}(z_1, z_2) \mid \varphi_{20}(z_2) \rangle$$

included in the optical potential $V(z_1)$. The second assumption means, that the functions

$$\varphi_n(z_1, z_2)$$

are obtained as normalized eigenvectors in a usual bound state shell model calculation. We shall for simplicity assumt that the energy scale is so, that E=0 for k=0, particle 2 in the state φ_{20}.

So we have

$$\langle \Psi^+(\kappa', z_1)\, \varphi_{20}(z_2) \mid H_{PP} \mid \Psi^+(\kappa, z_1)\, \varphi_{20}(z_2) \rangle = \frac{2}{\pi} E(\kappa)\, \delta'(\kappa - \kappa') \qquad (3.4)$$

$$\langle n \mid H_{QQ} \mid m \rangle = E_n \delta_{nm}. \qquad (3.5)$$

The projection operator P will in our case contain a projection operator

$$P_2 = \varphi_{20}(z_2) \int \varphi_{20}^*(z_2')\, dz_2' \qquad (3.6)$$

We can now from the Schrödinger equation get the usual set of coupled equations

$$(H_{PP} - E)\, P\Psi = -H_{PQ}\, Q\Psi \qquad (3.7)$$

$$($$

$$(H_{QQ} - E)\, Q\Psi = -H_{QP}\, P\Psi \qquad (3.8)$$

$$(H_{PQ} \equiv PHQ \quad , \quad H_{QP} \equiv QHP).$$

The first equation has the solution

$$P\Psi = G_P^+ H_{PQ}\, Q\Psi + \chi_P, \qquad (3.9)$$

where G_P^+ is the Green function for particle 1, corresponding to the optical model Hamiltonian, contained in H_{PP} (in general multiplied P_2), χ_P is a solution of

$$(H_{PP} - E)\, \chi_P = 0 \quad , \quad Q\chi_P = 0. \qquad (3.10)$$

It therefore obviously must have the form

$$\chi_P = c'(\kappa)\, \varphi_{20}(z_2)\, \Psi^+(\kappa(E), z_1). \qquad (3.11)$$

The expression for $P\Psi$ is now inserted in the second equation, to obtain

$$(H_{QQ} - E)\, Q\Psi + H_{QP}\, G_P^+ H_{PQ}\, Q\Psi + H_{QP}\, \chi_P = 0. \qquad (3.12)$$

We may now use the expressions (3.3) for $Q\Psi$ and (3.11) for χ_P multiply with $\varphi_m(z_1, z_2)$ from the left, and integrate over z_1, z_2 to obtain

$$\sum_n c_n \left[(E_n - E)\, \delta_{nm} + \iint dz_1\, dz_2\, \varphi_m H_{QP} G_P^+(E) H_{PQ}\, \varphi_n \right] +$$

$$+ c'(\kappa) \iint dz_1\, dz_2\, \varphi_m H_{QP}\, \varphi_{20}(z_2)\, \Psi^+(\kappa(E), z_1) = 0 \qquad (3.13)$$

$$\equiv \sum_n c_n \left[(E_n - E)\, \delta_{nm} + M_{nm}(\kappa) \right] + c'(\kappa)\, N_m(\kappa) = 0.$$

This equation, which is not an eigenvalue equation, since any $E(\kappa)$ in an allowed region gives solution, determines the c's up to a common normalization factor.

We see that the Green function $G^+(E)$, and the scattering state $\Psi^+(\kappa)$ both enter in this expression, respectively in M and N, multiplied with the residual interactions H_{PQ} and H_{QP} and integrated with bound state wave functions. Now, these latter go rapidly to zero with increasing z_1 and z_2, and the residual interactions are of finite range. We can therefore, with any desired accuracy replace the infinite integrals in M and N with integrals up to R, where R is of nuclear dimensions.

When this is done, we can introduce the MLE of $G_P^+(E(\kappa))$ and Ψ^G

$$G_P^+(\kappa) = \sum_n{}' \frac{\varphi_n(z_1) \varphi_n(z_1')}{2 K_n (\kappa - \kappa_n)} , \tag{3.14}$$

$$\Psi^{+G}(\kappa, z_1) = - \sum_n{}' \frac{\varphi_n(z_1) \varphi_n(R)}{2 K_n (\kappa - \kappa_n)} . \tag{3.15}$$

The easiest way to solve the system of equation thus obtained is presumably the following, suggested by Fano[21].

The matrix $(E_n - E(\kappa))\delta_{nm} + M_{nm}(k)$ is diagonalized by an energy dependent transformation, which carries our equation over into

$$c_\mu(k) (E_\mu(k) - E(\kappa)) + c'(k) N_\mu(k) = 0 \tag{3.16}$$

so

$$c_\mu(\kappa) = \frac{c'(\kappa) N_\mu(\kappa)}{E(\kappa) - E_\mu(\kappa)} . \tag{3.17}$$

The main part of the calculation is the diagonalization, which should be performed for all values of K. It is in this respect a great advantage, that our M_{nm} and N_m have the simple forms

$$M_{mn} = \sum_\ell{}' \frac{1}{2 k_\ell(\kappa - \kappa_\ell)} \int_0^R\int_0^R dz_1 dz_2 \, \varphi_m(z_1, z_2) H_{QP} \varphi_{2o}(z_1) \varphi_\ell(z_1) \times$$
$$\times \int_0^R\int_0^R dz_1 dz_2 \, \varphi_{2o}(z_2) \varphi_\ell(z_1) H_{PQ} \varphi_n(z_1, z_2) \tag{3.18}$$

(the $\varphi_n(z_1, z_2)$ are of course also of the form $\sum_{\ell_1 \ell_2}' c_{\ell_1 \ell_2}'' \varphi_{\ell_1}(z_1) \varphi_{\ell_2}(z_2)$)

$$N_m(\kappa) = -\sum_\ell{}' \frac{\varphi_\ell(R) e^{-ikR}}{2 k_\ell(\kappa - \kappa_\ell)} \int_0^R\int_0^R dz_1 dz_2 \, \varphi_m(z_1 z_2) H_{QP} \varphi_{2o}(z_2) \varphi_\ell(z_1) . \tag{3.19}$$

In calculation of the normalization constant it is not so advantageous to use the MLE.

We shall here, for our total wave function $\Psi(E(\kappa), z_1, z_2)$ use the same normalization as for $\Psi^+(k, z_1)$, i.e., we shall divide the coefficients with A, calculated from

$$\int_0^\infty\int_0^\infty dz_1 dz_2 \, \Psi^*(E(\kappa)) \Psi(E(\kappa')) = \frac{\pi}{2} \delta(\kappa - \kappa') |A|^2$$

$$= \int_0^\infty d\kappa'' c_\kappa^*(\kappa) c_{\kappa'}(\kappa'') + \sum_n{}' |c_n|^2 \tag{3.20}$$

here

$$c_\kappa(\kappa'') = \frac{2}{\pi} \int_0^\infty dz_1 \int_0^\infty dz_2 \, \Psi^{+*}(\kappa'', z_1) \varphi_{2o}(z_2) P \Psi$$

$$= \frac{2}{\pi} \int_0^\infty\int_0^\infty dz_1 dz_2 \, \Psi^{+*}(\kappa'', z_1) \varphi_{2o}(z_1) G_P^+(\kappa) H_{PQ} Q \Psi + \tag{3.21}$$
$$+ c'(\kappa) \delta(\kappa - \kappa'')$$

here, we shall use

$$G_P^+ = \frac{2}{\pi} \int_0^\infty \frac{d\kappa' \Psi^+(\kappa', z_1) \Psi^{+*}(\kappa', z_1')}{\kappa^{+2} - \kappa'^2} . \tag{3.22}$$

If, what in general will be the case , $H_{PQ} = H_{QP}^*$

$$c_\kappa(\kappa'') = \frac{1}{\kappa^2 - \kappa''^2} \sum_m c_m N_m^*(k) + c'(\kappa) \delta(\kappa - \kappa'') \tag{3.24}$$

and our normalization constant is determined by

$$\frac{\pi}{2} \delta(\kappa - \kappa') |A|^2 = \int d\kappa'' [c'(\kappa) \delta(\kappa - \kappa'') +$$
$$+ \frac{1}{\kappa^2 - \kappa''^2} \sum_m c_m N_m^*(\kappa)] \cdot [c'(\kappa)^* \delta(\kappa' - \kappa'') +$$
$$+ \frac{1}{\kappa'^2 - \kappa''^2} \sum_m c_m^* N_m(\kappa')] + \sum_n{}' c_n(\kappa) c_n^*(\kappa') \tag{3.25}$$
$$= |c'|^2 \delta(\kappa - \kappa') + \frac{\pi^2}{4\kappa^2} |\sum_m c_m N_m^*(\kappa)|^2 \delta(\kappa - \kappa')$$

so

$$|A|^2 = \frac{2}{\pi} |c'(\kappa)|^2 + \frac{\pi}{2\kappa^2} |\sum_m c_m N_m^*(\kappa)|^2 . \tag{3.26}$$

The qualitative picture, obtained in this way, has been discussed many times. The cross section of, e.g., elastic scattering, will, due to the residual interactions, get a large number of narrow resonances. Averaging over an energy interval, which is larger than these widths, one gets again back a cross section corresponding to the Ψ^+, however with somewhat larger single particle resonance widths.

A different situation is met, if the residual interaction has matrix elements mainly to such states, where the other degrees of freedom - in the above model represented by the particle 2-, takes up a small amount of the energy only. This will often

be the case with collective degrees of freedom. In such cases, the assumption of only one continuum must be given up, but on the other hand, the admixture of discrete states will be large only, when these states, as well as the total energy lies near the particle emission threshold.

As an extreme, but not unrealistic example one can think of the coupling of the single particle states to a static deformed field, as treated in ref.[22].

In such cases, the main effect of the residual interaction can be described as the shift of positions and widths of resonances.

A method to calculate these shifts in perturbation theory was given in ref.[23].

The starting point here is the Dyson relation between G_o^+ and G^+, pertaining to the unperturbed and the perturbed potential, respectively

$$G^+ = G_o^+ + G_o^+ H' G^+,\qquad (3.27)$$

where H' is the perturbation. Assuming again, that the perturbation is active inside R only, we can again introduce MLE for both G^+ and G_o^+. Equating the residues at $\kappa = \kappa_n$, one gets

$$\varphi_n = \sum_m{}' \frac{\varphi_m^o}{2 \kappa_m^o (\kappa_n - \kappa_m^o)} \int_0^R \varphi_m^o H' \varphi_n \, d\tau. \qquad (3.28)$$

If we put

$$\begin{aligned} H' &= \lambda u \\ \kappa_n &= \sum_{i=0} \lambda^i \kappa_n^{(i)} \\ \varphi_n &= \sum_{i=0} \lambda^i \varphi_n^{(i)} \end{aligned} \qquad (3.29)$$

and equate the coefficients of each power of λ, one gets a perturbation series for wave functions and energies.

It should be noted, however, that there is no term by term correspondence between these series, and the usual perturbation series, even when we look at the contributions from bound state residua only. This is due to the nonorthogonality of the resonance functions. Only the 1. order corrections in the energy are in agreement. If an exact diagonalization in a truncated space is preferred, a similar problem is met. The equation

$$(H - E) \Psi_{trunc} = (H_o + H' - E) \sum_n^N c_n \varphi_n = 0 \qquad (3.30)$$

leads, e.g., to a matrix eigenvalue equation, when multiplied by N independent functions and integrated over all angles and over r from 0 to R.

Due to the non-orthogonality, E will appear with nondiagonal terms as well as diagonal between two bound states, its non diagonal contributions will be small, so that such eigenvectors which consist mainly of bound state components must resemble the usual ones. In general the non-diagonal terms are, however large. The non-orthogonality is not merely a calculational inconveniency, but also leads to a freedom in the choice of the set of equations, satisfied by the eigenvectors. A natural choice seems to be to assume that a certain basis $n = n_1 \ldots n_N$ is sufficient for the expansion of Ψ, and that the same basis functions are used for the matrix $\langle n_1 | H | n_2 \rangle$. It should be noted, that states with different ℓ-values are trivially orthogonal, and that therefore in the approximation of one pole for each ℓ-value in the expansion, no problem of the type mentioned arises[22].

The ambiguity in the choice of a truncated problem, is connected with the well-known absence of minimum principles for scattering states. However, stationarity principles do exist, and a better starting point for the truncation is obtained when we start from a stationary expression, and make a truncation of that expression. Now, the expression (3.27) above can just be obtained from the variation of an expression for

$$G^+ - G_o^+ = G_o^+ H' G^+$$

$$\delta(G_o^+ H' G^+ + G^+ H' G_o^+ - G^+ H' G^+ + G^+ H' G_o^- H' G^+) = 0, \qquad (3.31)$$

where the variation is in the parameters of G^+.

Since the expression is stationary, a small change in these parameters, like a truncation with sufficiently many terms must lead to an expression, which is near to the true one. Making now our variation with such a truncated expression, we obtain the equation

$$\sum_n^N c_n \varphi_n = \sum_m^{\infty} \frac{\varphi_m}{2 \kappa_m (\kappa - \kappa_m)} \int \varphi_m H' \left(\sum_n^N c_n \varphi_n \right) d\tau \qquad (3.32)$$

or, defining $\widetilde{\varphi}_m = \varphi_m / \sqrt{\kappa_m}$, $\widetilde{c}_m = \sqrt{\kappa_m}\, c_m$

$$\sum_m^N \widetilde{c}_m \widetilde{\varphi}_m = \sum_m{}' \frac{\widetilde{\varphi}_m}{2(\kappa - \kappa_m)} \int \widetilde{\varphi}_m H'\left(\sum_n \widetilde{c}_n \widetilde{\varphi}_n\right) d\tau . \qquad (3.33)$$

Equating the coefficients of $\widetilde{\varphi}_n$ we get

$$(\kappa - \kappa_m)\widetilde{c}_m = \sum_n \widetilde{c}_n \langle \widetilde{\varphi}_n^* H' \widetilde{\varphi}_m \rangle \qquad (3.34)$$

which is obviously an eigenvalue problem of the usual type, though non-Hermitian (but symmetric). In general, the overcompleteness of the φ's must mean, that the leaving out, from the truncated basis of some of the functions is less dangerous than with the usual expansion methods. In practice, looking for resonances in G^+ we can exclude from our basis all such components which, if they were large, would lead to a non-resonant behaviour, i.e., the antibound functions, the functions with negative $Re(\kappa_n)$ and the functions with $\Gamma \gg \kappa^2$.

In conclusion , it should be noticed, that numerical investigations of the MLE of the S-matrix are nearly absent in the literature (see though, the article by Weidenmüller[24]),and for the wave functions, such investigations were never carried out. In a forthcoming paper, as an illustration of the general results obtained above, we shall discuss numerical investigations for some simple potentials.

A p p e n d i x

It is easy to prove that the real poles are single, but somewhat more complicated to exlude multiple complex poles.

This is in the literature often done by arguing that such poles are a very rare phenomenon, which will only be seen for particular potentials.

This argumentation seems in need of a firmer, quantitative basis, which we shall here attempt to construct.

For all potentials with parameters, which can be varied in such a way that the poles are moving, the complex poles will become real by meeting pairwise at 0, for $\ell \neq 0$, or on the negative imaginary κ-axis, for $\ell = 0$. These double poles, which can be avoided by a slight change of the parameters of the

potentials, are , for the potentials of relevance in nuclear physics, essentially the only ones.

The resonance condition (2.8) will lead to a multiple resonance if

$$\frac{d}{d\kappa}\left[\frac{\frac{d}{d\imath}\varphi_n(\imath)}{\varphi_n(\imath)}\right]_{\imath=R}\Bigg|_{\kappa=\kappa_n} = \frac{d}{d\kappa}\left[\frac{\kappa\, h_\ell^{+\,'}(\kappa R)}{h_\ell^+(\kappa R)}\right]_{\kappa=\kappa_n} . \qquad (A1)$$

In this case, the normalization condition (2.9) cannot be fulfilled , since (A1) leads to the identity

$$\int_0^R \varphi_n^2 \, d\imath + \frac{\varphi_n^2(R)}{2\kappa_n}\left[\frac{d}{d\kappa}\left(\frac{\kappa\, h_\ell^{+\,'}(\kappa R)}{h_\ell^+(\kappa R)}\right)\right]_{\kappa=\kappa_n} = 0 . \qquad (A1a)$$

Let us now consider a square well

$$\begin{aligned} V(\imath) &= 0 & \text{for} \quad \imath > R \\ V(\imath) &= -V_o & \text{for} \quad \imath \leqslant R \end{aligned} \qquad R = 1 \qquad (A2)$$

then

$$\varphi = const \cdot j_\ell(K) \qquad (A3a)$$

with

$$K = (\kappa^2 + V_o)^{1/2} . \qquad (A3b)$$

The resonance condition (2.8) is now

$$\kappa \frac{d}{d\kappa}\left[\ell n(h_\ell^+(\kappa))\right]_{\kappa=\kappa_n} = K \frac{d}{dK}\left[\ell n(j_\ell(K))\right]_{K=K(\kappa_n)} \qquad (A4)$$

and the condition (A1) that it is a multiple pole, is

$$\frac{d}{d\kappa}\left[\kappa \frac{d}{d\kappa}(\ell n(h_\ell^+(\kappa)))\right]_{\kappa=\kappa_n} = \frac{d}{d\kappa}\left[K\frac{d}{dK}(\ell n(j_\ell(K)))\right]_{K=K_n} \qquad (A5)$$
$$(K=K(\kappa))$$

or

$$\kappa \frac{d^2}{d\kappa^2}(\ell n(h_\ell^+(\kappa))) + \frac{d}{d\kappa}(\ell n(h_\ell^+(\kappa))) =$$
$$= K\frac{d^2}{dK^2}(\ell n(j_\ell(K))) + \frac{K}{\kappa}\frac{dK}{d\kappa}\frac{\kappa}{K}\frac{d}{dK}(\ell n(j_\ell(K))) \qquad (A6)$$
$$K = K(\kappa) \quad , \quad \kappa = \kappa_n .$$

Now, we can use the Riccatti-Bessel equation, satisfied by $z = h_\ell^+$ and $z = j_\ell$

$$\frac{d^2}{d\rho^2}(\ell n(z(\rho))) + \left(\frac{d}{d\rho}(\ell n(z(\rho)))\right)^2 = \frac{\ell(\ell+1)}{\rho^2} - 1 \qquad (A7)$$

and

$$\frac{K}{k}\frac{dK}{d\kappa} = 1 \tag{A8}$$

(seen from (A3b))
to transform this into

$$\kappa \left\{ -\frac{\ell(\ell+1)}{\kappa^2} - 1 - \left[\frac{d}{d\kappa}\left(\ln\left(h_\ell^+(\kappa)\right)\right)\right]^2 - \right.$$

$$- \frac{\ell(\ell+1)}{K^2} + 1 + \left[\frac{d}{dK}\left(\ln\left(j_\ell(K)\right)\right)\right]^2 \right\} + \tag{A9}$$

$$+ \frac{d}{d\kappa}\left(\ln\left(h_\ell^+(\kappa)\right)\right) - \frac{\kappa}{K}\frac{d}{dK}\left(\ln\left(j_\ell(K)\right)\right) = 0 \quad \begin{matrix} K = K(\kappa) \\ \kappa = k_n \end{matrix}$$

or, using (A4)

$$-\frac{V_0}{K^2}\left\{\frac{d}{d\kappa}\left[\ln\left(h_\ell^+(\kappa)\right)\right] + \frac{\ell(\ell+1)}{\kappa} - \kappa\frac{d}{d\kappa}\left[\ln\left(h_\ell^+(\kappa)\right)\right]\right\} \tag{A10}$$

or

$$\frac{d}{d\imath}\left(\ln\left(\varphi_n\right)\right)\Big|_{\imath=1} = \kappa\frac{d}{d\kappa}\left(\ln\left(h_\ell^+(\kappa)\right)\right)\Big|_{\kappa=k_n} = \begin{cases} -\ell \\ \ell+1 \end{cases} \tag{A11}$$

which could not be fulfilled for a complex pole, since, e.g.,

$$Im\left[\frac{d}{d\imath}\ln\left(\varphi_n\right)\right]_{\imath=1} = -\Gamma_n\frac{\int_0^1|\varphi_n|^2 d\imath}{|\varphi_n(1)|^2} < 0 \tag{A12}$$

for a real potential.

Now with the normalization (2.9), the shift of a pole position, δE_n for a small change of the potential, δV is given by the usual perturbation expression

$$\delta E_n = \int \varphi_n^2 \, \delta V \, d\tau \tag{A13}$$

(cf. eq. (3.29)).

This perturbation approach, which presupposes that the poles are single, will converge and lead to a new potential with non-degenerate eigenvalues, provided $|\delta E_n|$ is smaller than $|E_n - E_j|$ for all E_j .

In nuclear physics, the Woods-Saxon potential is the most used. This is strictly speaking different from zero for all r-values. For the present purpose it is, however, completely legitimate to replace it by zero outside R, provided this is chosen well beyond the nuclear radius.

This potential will also, for all practical applications, deviate from a square well by a δV which fulfills the above requirement.

R e f e r e n c e s

1. C.Mahaux and H.A.Weidenmüller, Shell-Model Approach to Nucklear Reactions, Amsterdam, North-Holland, 1969.
2. L.Eisenbud and E.P.Wigner, Phys.Rev. 72 (1947) 29.
3. P.L.Kapur and R.E.Peierls, Proc.Roy.Soc. A166 (1938) 277.
4. K.Meetz, Journ.Math.Phys. 3 (1962) 690.
5. T.Sasakawa, Nucl.Phys. A160 (1971) 321.
6. J.M.Bang and F.A.Gareev, Preprint JINR, E2-10624, 1977.
7. J.M.Bang and F.A.Gareev, Preprint JINR, E2-10625, 1977.
8. G.Gamow, Z.Phys. 51 (1928) 204.
9. R.E.Peierls, Proc.Roy.Soc. A253 (1959) 16.
10. J.Humblet and L.Rosenfeld. Nucl.Phys. 26 (1961) 329.
11. Ya.B.Zel'dovich. JETP (Sov.Phys.) 12 (1961) 542.
12. T.Berggren, Nucl.Phys. A109 (1968) 265.
13. W.Romo, Nucl.Phys. A116 (1968) 618.
14. G.Garcia-Calderon. Nucl.Phys. A261 (1976) 130.
15. G.Garcia-Calderon and R.Peierls, Nucl.Phys. A265 (1976) 443.
16. H.M.Nussenzveig, "Causality and Dispersion Relations", Academic Press, New York, 1972.
17. B.I.Serdobol'skij, JETP, 36 (1959) 1903.
18. J.R.Taylor. Scattering Theory, New York, John Wiley, 1972.
19. V.de Alfaro and T.Regge, Potential Scattering, Amsterdam, North-Holland, 1965.
20. J.Block et al. Rev.Mod.Phys. 23 (1951), 147.
21. U.Fano, Phys.Rev. 124 (1961), 1866.
22. J.Bang, F.A.Gareev, J.V.Puzynin and R.M.Jamalejev. Nucl. Phys. A261 (1976) 59.
23. R.M.More and E.Gerjuoy, Phys.Rev. A7 (1975) 1188.
24. H.A.Weidenmüller, Ann. of Phys. 28 (1964) 60.
25. J.Bang and J.Zimanyi, Nucl.Phys. A139 (1969) 534.