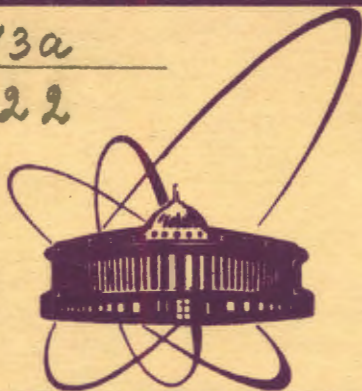


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A NEW TYPE OF REAL WEINBERG FUNCTIONS

Объединенный институт
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Новый вариант действительных функций Вайнберга

Показана возможность введения действительных функций Вайнберга для любых фазовых сдвигов. Рассмотрены разложения по данным функциям К-матриц, функций Грина, волновых функций непрерывного спектра. Показана равномерная сходимости данных разложений. Установлено, что сходимости разложений наилучшая, когда фазовый сдвиг равняется фазовому сдвигу потенциального рассеяния. Результаты работы демонстрируются на примере потенциала прямоугольной ямы.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна 1979

Bang J., Ershov S.N., Gareev F.A.

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A New Type of Real Weinberg Functions

The concept of real Weinberg states is generalized to arbitrary phase shifts. Expansions in terms of such states are investigated mathematically and numerically. Such expansions are shown, in some important cases, to have particularly convenient convergence properties.

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

Communication of the Joint Institute for Nuclear Research. Dubna 1979

1. INTRODUCTION

The complex Weinberg states were introduced by Meetz ^{1/} and Weinberg ^{2/} as a means of improving the convergence of the Born approximation in elastic single particle scattering and, hopefully, other scattering problems. These states are eigensolutions of a Lippman-Schwinger equation (with outgoing boundary conditions).

The completeness of these states, for well behaved potentials, was proved by means of analytic continuation from the corresponding expansion negative energy, the Sturm-Liouville expansion, which by Mercer's theorem is shown to be absolutely and uniformly convergent.

Real Weinberg states were introduced by Huby ^{3/} and Sasakawa ^{4/}. These states are eigensolutions of a similar problem as the original Weinberg states, but with real boundary conditions for $r \rightarrow \infty$ corresponding to those of a scattering state (phase shift $\Delta = \frac{\pi}{2}$).

The eigenvalues are therefore also real. It should, though, be noted that they can have both signs ^{5/}. For the potentials of physical interest, mentioned below, however, only a finite number of the eigenvalues are negative, and Mercer's theorem may be used in a direct way to prove completeness.

Although these real Weinberg expansions are not so directly tied up with the scattering problems as the original complex states, they can in general be used in a similar way, constructing the S matrix from the K-matrix.

We shall in this article look at a more general definition of real Weinberg states, corresponding to those of Huby and Sasakawa, but with arbitrary values of the phase shift. For the potentials of interest also these states form a complete set, and most of the properties of the above-mentioned states with $\delta = \frac{\pi}{2}$ find their

counterparts in the general case. It is not surprising,

that the states with $\delta = \frac{\pi}{2}$ work well as an expansion

basis in the neighbourhood of a single particle resonance of the relevant particle; therefore, e.g., Huby could calcu-

late an important part of the cross section of continuum transfer, using only one real Weinberg state. However, in other cases, far from resonances, other boundary conditions may lead to a considerably better convergence of the expansions, as we shall see below.

2. FORMALISM

The generalized real Weinberg functions can be defined as the solutions of

$$(H_0 + \gamma V(r) - E)\phi^\Delta = 0, \quad (1)$$

$$\phi^\Delta = \frac{f_\ell^\Delta}{r} Y_{\ell m}(\Omega)$$

with E given, and γ as eigenvalue with the boundary conditions

$$f(0) = 0, \quad (2)$$

$$f(r) \xrightarrow{r \rightarrow \infty} F(r) \sin(\Delta) + G(r) \cos(\Delta), \quad (3)$$

where F and G are regular and irregular solutions, respectively, of the radial Schrödinger equation.

In equation (1) H_0 includes the kinetic energy operator, but it may also be convenient to let it include possible Coulomb repulsion and spin-orbit terms. The first because the Coulomb field is of infinite range, and known, i.e., it gives a known contribution to the asymptotic behaviour of the wave functions. The spin orbit term is neither positive nor negative definite. By including these terms in H_0 , we may limit ourselves to a negative definite, finite V of finite range, as, e.g., the Woods-Saxon potential or its square well variant.

For a finite range potential, (3) can also be written

$$f(r) \xrightarrow{r \rightarrow \infty} \sin(kr + \Delta) \quad \left(\frac{\hbar^2 k^2}{2m} = E \right). \quad (4)$$

The functions of Huby and Sasakawa correspond to the choice $\Delta = \frac{\pi}{2}$.

If

$$V(r) = 0 \quad \text{for } r > a, \quad (5)$$

we can instead of (4) write

$$f_\ell(r) = c \hat{j}_\ell(kr + \Delta) \quad r > a, \quad (6)$$

where \hat{j}_ℓ is a Ricatti-Bessel function. In this case, the set of eigensolutions, f_i , of (1) with the boundary conditions (2)-(6), corresponding to different γ_i form, as shown by Kato^{8/}, a complete set in the interval $(0, a)$. They are orthogonal with the weight function $V(r)$, i.e.,

$$\int_0^a dr f_n V f_m = \delta_{nm} a_n \quad (7)$$

and may be normalized by putting $a_n = -1$.

The completeness relation may be written

$$\begin{aligned} \sum_i V^{1/2}(r) f_i(r) f_i(r') V^{1/2}(r') &= \\ &= -\delta(r-r') \\ &= -\sum_i V(r) f_i(r) f_i(r') \\ &= -\sum_i f_i(r) f_i(r') V(r'). \end{aligned} \quad (8)$$

In general, the different forms of (8) correspond to slightly different spaces, for bounded functions in the interval $(0, a)$ they are, however, all valid with the potentials in which we are interested.

Using the completeness relation, we can write the Green function, corresponding to the asymptotic behaviour of the second term in a Lippman-Schwinger-like equation being given by (4) as

$$G_\ell^\Delta(r, r') = -\sum_n \frac{1}{\gamma_n - 1} f_{\ell n}^\Delta(r) f_{\ell n}^\Delta(r') \quad \left(\frac{\hbar^2 k^2}{2m} = E \right). \quad (9)$$

The Schrödinger equation

$$(H + V - E)\psi = 0 \quad (10)$$

of a general scattering problem has solutions ψ^+ , which describe scattering from an initial channel, say a , in which we have a normalized free particle wave function, ψ_0

$$\psi^+ = \psi_0 + G^+ V \psi_0 \quad (11)$$

but equation (10) has other solutions, with other boundary conditions, e.g.,

$$\psi^\Delta = \psi_0 + G^\Delta V \psi_0, \quad (12)$$

where the second term behaves asymptotically as ϕ^Δ . Here, Δ may take different values in different channels, and in (12) and the following equations, we shall think of Δ as an operator, operating on channel indices.

Equations (11) and (12) may also be written, respectively as

$$\psi^+ = \psi_0 + G_0^+ V \psi^+ \quad (13)$$

and

$$\psi^\Delta = \psi_0 + G_0^\Delta V \psi^\Delta. \quad (14)$$

Here

$$\begin{aligned} G_0^\Delta &= G_0^+ - \frac{e^{-i\Delta} \pi}{\sin(\Delta)} \delta(E - H_0) = \\ &= G_0^+ - \frac{e^{-i\Delta} \pi}{\sin(\Delta)} \sum_{\beta} \psi_{0\beta}(E) \langle \psi_{0\beta}(E) | \end{aligned} \quad (15)$$

where the sum runs over the different channels in scattering (characterized by spins, etc.).

Subtracting (13) from (14) we get, using (15)

$$\begin{aligned} \psi_a^\Delta - \psi_a^+ &= D\psi = G_0^\Delta V D\psi - \frac{\pi e^{-i\Delta}}{\sin(\Delta)} \delta(E - H_0) V \psi_a^+ \\ &= G_0^\Delta V D\psi - \sum_{\beta} \frac{e^{-i\Delta\beta} \pi}{\sin(\Delta\beta)} \psi_{0\beta} \mathcal{J}_{\beta a} \\ &= - \sum_{\beta} \frac{e^{-i\Delta\beta} \pi}{\sin(\Delta\beta)} \psi_{\beta}^\Delta \mathcal{J}_{\beta a}, \end{aligned} \quad (16)$$

where ψ_0 belongs to the channel a , and

$$\mathcal{J}_{\beta a} = \langle \psi_{0\beta} V \psi_a^+ \rangle. \quad (17)$$

Introducing

$$K_{\beta a}^\Delta = -\pi \langle \psi_{0\beta} V \psi_a^\Delta \rangle \quad (18)$$

we see, that for the T-matrix we have

$$\pi T = -K^\Delta - \frac{e^{-i\Delta} \pi}{\sin(\Delta)} K^\Delta T. \quad (19)$$

So

$$\pi T = - \left(1 + \frac{e^{-i\Delta}}{\sin(\Delta)} K^\Delta \right)^{-1} K^\Delta \quad (20)$$

and

$$S = 1 - 2\pi i T = \left(1 + \frac{e^{-i\Delta}}{\sin(\Delta)} K^\Delta \right)^{-1} \left(1 + \frac{e^{i\Delta}}{\sin(\Delta)} K^\Delta \right) \quad (21)$$

for the usual K-matrix we get

$$K = \frac{\pi T}{i\pi T - 1} = (1 + \cot(\Delta) K^\Delta)^{-1} K^\Delta. \quad (22)$$

So all the useful quantities of scattering theory may be derived from K^Δ , which in turn may be expressed by means of the generalized real Weinberg states, since, from (18) and (9) we get for the K^Δ -operator

$$K^\Delta = -\pi(V + VG^\Delta V) = -\pi(V - \sum_n \frac{1}{\gamma_n - 1} V|\phi_n^\Delta\rangle\langle\phi_n^\Delta|V). \quad (23)$$

Using (8) and introducing the Lippman-Schwinger eigenvalue

$\lambda_n = \gamma_n^{-1}$ equation (23) may also be written

$$K^\Delta = \pi \sum_n \frac{V|\phi_n^\Delta\rangle\langle\phi_n^\Delta|V}{1 - \lambda_n^\Delta}. \quad (24)$$

Looking at elastic scattering, we see from (21), with $S_{\ell\ell} = e^{2i\delta_\ell}$, that for $\Delta = \Delta_\ell \rightarrow \delta_\ell \cdot (+\pi)$ we must have $K_{\ell\ell}^\Delta \rightarrow \infty$, except possibly for the case of $\delta_\ell = n\pi$. This is in agreement with (1), (4) and (24), since $\gamma_i^\Delta \rightarrow 1$ ($\lambda_i^\Delta \rightarrow 1$) for a certain i when $\Delta \rightarrow \delta$, expect for $\Delta \rightarrow 0$, where $\gamma_i^\Delta \rightarrow 0$ ($\lambda_i^\Delta \rightarrow \infty$).

3. APPLICATIONS

The variant of the real Weinberg states, which is proposed here, may be used in different sorts of nuclear reaction calculations, in the same way as the other types of Weinberg states. The advantage of the present type of states is, that if we are looking at a general scattering problem, and use our states as expansion basis of the solution, we know, roughly speaking, that if the expansion is good inside the range of the potential, and if the phase shifts correspond to these of the true solution, then the expansion is equally good in all regions of space. A similar feature is met with the "Natural Boundary Conditions" wave functions of Danos and Greiner¹¹, however in general, this expansion will depend on the cut-

off radius, whereas the Weinberg expansion will depend on this only when it is found necessary to truncate the potential at $r=a$ (see equation (5)). Such a truncation may be convenient for mathematical and numerical reasons, but for the Woods-Saxon potential the expansion is independent of a , when a is sufficiently large.

If we expand a function, which satisfies a radial Schrödinger equation with the same energy and the same phase shift as that of the basis functions, i.e., looking at the radial equation, corresponding to (10)

$$(H_0 + \gamma V + V_1 - E)f = 0, \quad (25)$$

$$f = \sum_n c_n f_n. \quad (26)$$

$$c_n = -\int_0^a f V f_n dr = \lambda_n \int_0^a dr f (H_0 - E) f_n = -\gamma_n^{-1} \int_0^a dr f (\gamma V + V_1) f_n = (\gamma - \gamma_n)^{-1} \int_0^a f V_1 f_n dr. \quad (27)$$

$$= (\gamma - \gamma_n)^{-1} \int_0^a f V_1 f_n dr. \quad (28)$$

Now, $\gamma_n \sim n^2$ and the integrals must go to zero for $n \rightarrow \infty$, so the expansion converges faster than n^{-2} .

The absolute and uniform convergence, which by Mercer's theorem is proved to be valid for $r < a$, is in this case extended to all r -values, and this result is independent of a .

The real advantages of the Weinberg expansions are seen in multichannel scattering, but the convergence properties of the one-dimensional problem of equations (25) to (28) must also be found here. The choice of the phase shifts of the basis, is presumably the most intricate problem of the method suggested, as well as of the Natural Boundary Condition model. If experimental phase shifts are known, a logical method would be to use these in the basis, and then search for such values of free parameters of the Hamiltonian, that the total scattering wave function has the same phase shift.

It is in this connection interesting to see, how the expansion of a scattering wave function converges, when the phase shifts of the basis are varied. In the figure

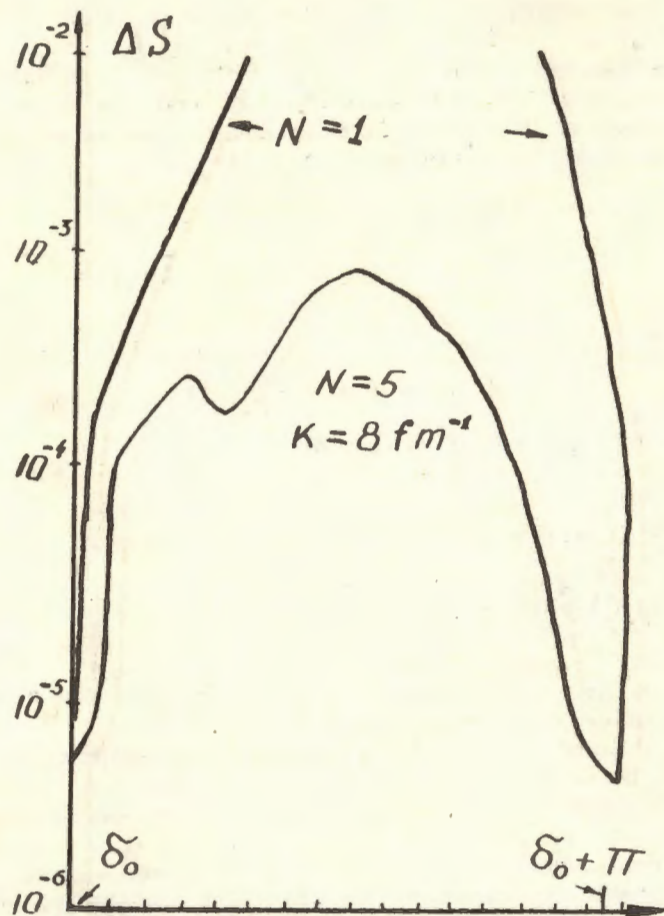


Fig. The relative error of S , as a function of Δ . N is the number of terms in the expansion.

we present a calculation for the one-dimensional case. The potential is a square well with parameters similar to those used in nuclear physics, and the states have $l=0$. The figure shows the relative errors of the scattering matrix

$$\Delta S = \left| \frac{S - S_{\text{exact}}}{S_{\text{exact}}} \right|, \quad (29)$$

where S is calculated by the expressions (19)-(24), using respectively 1 and 5 terms in the expansion. The potential depth is -48.72 MeV, the radius parameter

$\beta_0 = R_0 \left(\frac{2m}{\hbar^2} |V_0| \right)^{1/2}$ is 5.0, the energy corresponds to $k = 8 \text{ fm}^{-1}$.

It is seen, that the errors become vanishingly small when Δ approaches δ_0 and $\delta_0 + \pi$, where δ_0 is the elastic phase shift for the potential and energy given above but it is also seen, that with 5 terms in the expansion, the error is small for all Δ values. This means, that even if the starting values of Δ are not very good, exactness is not lost, when a moderate number of terms is used in the expansion.

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