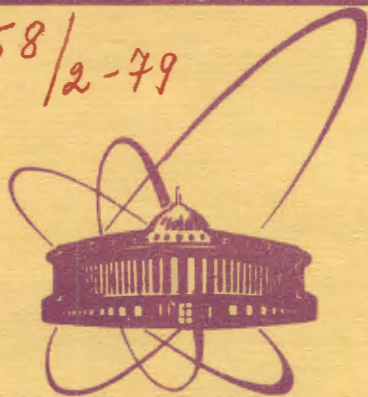


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**J.Bang , S.N.Ershov, F.A.Gareev, G.S.Kazacha**

**DISCRETE EXPANSIONS  
OF CONTINUUM WAVE FUNCTIONS.  
NUMERICAL EXAMPLES**

**1979**

Банг Е. и др.

E4 - 12611

Дискретные разложения волновых функций континуума.  
Численные примеры

Данная работа является окончанием серии статей (I, II)<sup>1)</sup>, посвященных дискретным разложениям волновых функций континуума в конечной области пространства. В работе проводится численное исследование сходимости Вайнберговских разложений для  $S, K$  матриц, волновых функций непрерывного спектра. Рассматривается случай одночастичных состояний континуума для потенциалов Саксона-Вудса и прямоугольной ямы. Обсуждаются некоторые численные методы для решения задач на собственные значения встречающихся в данных разложениях.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Сообщение Объединенного института ядерных исследований, Дубна 1979

Bang J. et al.

E4 - 12611

Discrete Expansions of Continuum Wave Functions.  
Numerical Examples

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

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## 1. Introduction

In two preceding papers (I, II)<sup>1)</sup> different discrete expansions of continuum wave functions in a finite region were reviewed. Particular attention was paid to the Mittag-Leffler and Weinberg expansions.

In this paper, where we use common notation with I, II, we investigate the convergence of the Weinberg expansions, particularly the real Weinberg expansions, numerically. We look at the case of single particle continuum states and corresponding  $S$ -matrices, with square well and Woods-Saxon potentials.

A new type of real Weinberg states, proposed in I, is shown to give expansions with particularly convenient convergence properties. Some numerical methods for solving the eigenvalue problems, corresponding to the different expansions, are discussed in the Appendix.

## Numerical Results

In the same way as it was shown for the bound state Sturm-Liouville case<sup>2)</sup>, it can be shown, that all the eigenvalues mentioned above, which have the dimension of an energy for large values of the radial quantum number,  $\Omega$ , will behave as  $\Omega^2$ . That means, that  $K_n \sim \Omega$  (Kapur-Peierls or KPC),  $\lambda_n$  (Sturm-Liou-



ville, real and complex Weinberg)  $\sim \frac{1}{k}$ . Note, that we have here, in agreement with refs. 3,4) introduced  $\lambda_n \equiv \lambda_n^{LS} = 1/\delta_n$ , the Lippman-Schwinger eigenvalue, whereas the Sturm-Liouville eigenvalue of ref. 2) was defined as  $\lambda_n^{SL} \equiv \lambda_n^{SL} = \chi_n$ .

In fig. 1, the eigenvalues  $\lambda_n^{SL} = \chi_n$ ,  $\ell = 0$  for a square well are shown as a function of  $K$ . Note, that the minor of posi-

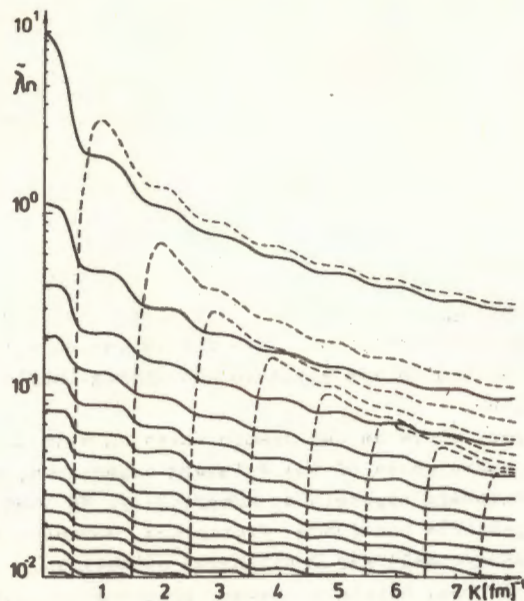


Fig. 1. The  $k$ -dependence of the eigenvalues  $\lambda_n (\Delta = \frac{\pi}{2})$  of the real Weinberg functions for the rectangular well with  $V_0 = -48.72$  MeV,  $R_0 = R_0 \left( \frac{2m}{\hbar^2} |V_0| \right)^{\frac{1}{2}} = 5.0$ . The full curves denote the positive  $\lambda_n$ ; the dotted, the negative  $\lambda_n$ .

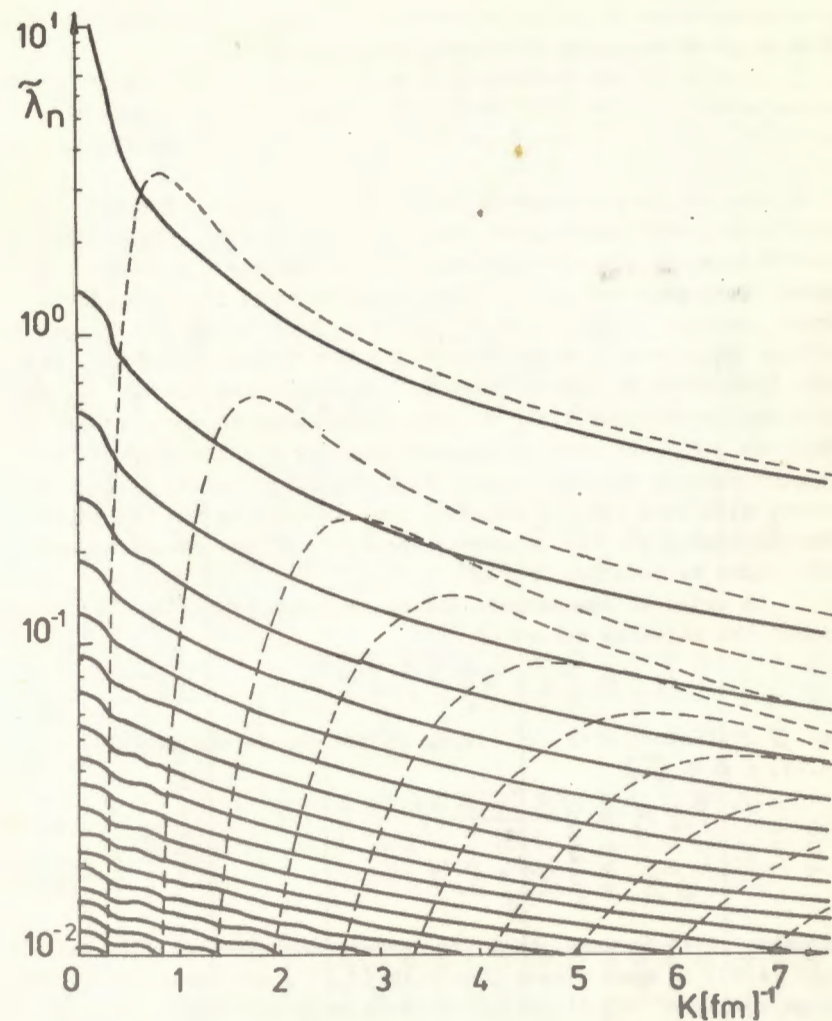


Fig. 2. The  $k$ -dependence of the eigenvalues  $\lambda_n (\Delta = \frac{\pi}{2})$  of the real Weinberg states of the Woods Saxon potential with the parameters of the text. Symbols as in fig. 1.

tive eigenvalues is infinite for all  $K$  values, the number of negative eigenvalues is an increasing function of  $K$ .

In fig. 2 the corresponding eigenvalues with a cut-off Woods-Saxon potential,  $V = -V_0(1 + \exp((r-R)/\alpha))^{-1}$ ,  $R = 3.26$  fm,  $\alpha = 0.63$  fm,  $V_0 = 53.35$  MeV, are shown. Note, that the oscillation of fig. 1 disappears for the more smooth potential.

Due to the presence of the factors  $\lambda_n$  the expansions (4.8), etc., must converge at least as fast as  $\frac{1}{n^2}$ . Note, that (4.21) does not contain the factor  $\lambda_n$ , whereas (4.20) does. It should further be mentioned that in integrals, containing the Green operator (4.8) or the  $K$ -operator (4.21), the oscillations of the  $\varphi_n$ , which become more rapid for larger  $n$ -values, will also contribute to the convergence, so that, like in ref.<sup>2)</sup>,  $\frac{1}{n^2}$  is actually an upper limit for the convergence of such integrals. That the  $\varphi_n$  are oscillating more rapidly for higher  $n$  values, is particularly obvious for the real Weinberg states, it is, however, also true for the ordinary ones as well as for the Kapur-Peierls states and the resonance functions of the preceding section, when we consider  $r \leq a$ .

In order to demonstrate the convergence properties, we have listed the relative errors of

$$K = (K|K|K) \quad (4.28)$$

and  $S$ , obtained with  $N$  terms in the expansions (4.20) and (4.21) ( $\Delta = \frac{1}{2}$ )

$$\Delta K = \left| \frac{K^N - K}{K} \right| \quad (4.29)$$

$$\Delta S = \left| \frac{S^N - S}{S} \right| \quad (4.30)$$

in table 1. It is seen, that the convergence obtained with expression (4.20) is much slower than with (4.21), and particularly for large values of  $K$ , (4.20) is rather slowly convergent. This seems to be the reason, why the authors of ref.<sup>5)</sup> claim, that the basis of real Weinberg states is useless for higher energies. It is seen that the corresponding relative errors of the  $S$ -values follow the same pattern as for  $K$ , but that they are in general smaller. Since  $S$  is here obtained from a Hermitian  $K$ -matrix, it is unitary, independent of the number of terms in the expressions (4.20) or (4.21).

Table 1. The relative errors  $\Delta K_1(\Delta K_2)$  and the corresponding  $\Delta S_1(\Delta S_2)$ , calculated by means of equations 4.21 (4.20).  $\Delta \varphi$  and  $\Delta \psi$  are the mean error and the maximal error of the scattering wave functions, calculated by expansions in terms of real Weinberg states for the square well potential with the parameters  $R=1$  fm and  $V_0 = 20.75$  MeV.

$K$ (fm <sup>-1</sup> )	$\lambda_n$	$\Delta K_1$ $\Delta K_2$ $\Delta S_1$ $\Delta S_2$ $\Delta \varphi$ $\Delta \psi$							
		1	2	3	4	5	6	7	8
0.1	4.0365-01	3.62-04	9.13-03	4.00-05	1.01-03	2.61-04	4.99-04		
	4.5009-02	1.43-05	1.40-03	1.58-06	1.55-04	3.32-05	7.53-05		
	1.6209-02	1.42-06	4.32-04	1.57-07	4.78-05	8.69-06	2.24-05		
	8.2719-03	3.45-06	1.86-04	3.82-07	2.06-05	3.20-06	9.01-06		
	5.0031-03	3.91-06	9.45-05	4.33-07	1.04-05	1.48-06	4.38-06		
	3.3469-03	4.08-06	4.41-05	4.51-07	4.88-06	8.67-07	2.68-06		
1.0	2.6369-01	1.27-03	3.54-02	8.24-04	2.30-02	3.78-03	7.21-03		
	4.1434-02	7.87-05	6.57-03	5.08-05	4.24-03	5.54-04	1.30-03		
	1.5691-02	9.41-06	2.15-03	6.08-06	1.38-03	1.51-04	4.12-04		
	8.1344-03	2.29-07	9.64-04	1.48-07	6.23-04	5.67-05	1.74-04		
	4.9531-03	2.41-06	5.24-04	1.55-06	3.38-04	2.59-05	8.68-05		
	3.3281-03	3.03-06	3.36-04	1.96-06	2.17-04	1.34-05	4.91-05		
2.0	9.1366-02	2.57-02	6.42-01	1.41-02	3.66-01	1.55-02	7.32-02		
	4.3316-02	5.81-04	3.52-02	3.19-04	1.94-02	2.21-03	4.03-03		
	2.0197-02	7.23-05	1.00-02	3.97-05	5.52-03	4.90-04	1.08-03		



1	2	3	4	5	6	7	8
	9.2219-03	1.80-05	4.17-03	9.93-06	2.29-03	1.70-04	4.34-04
	5.3406-03	7.00-06	2.09-03	3.84-06	1.15-03	7.49-05	2.09-04
	3.4969-03	3.87-06	1.20-03	2.12-06	6.60-04	3.81-05	1.13-04
3.0	-1.3393-01	2.23-02	2.91-01	7.08-03	9.29-02	2.67-02	4.62-02
	8.1003-02	3.10-04	1.95-02	9.83-05	6.19-03	1.42-03	3.05-03
	1.9297-02	3.33-05	5.19-03	1.05-05	1.64-03	3.10-04	7.90-04
	9.0031-03	5.62-06	2.11-03	1.78-06	6.69-04	1.06-04	3.09-04
	5.2656-03	7.33-08	1.05-03	2.32-08	3.34-04	4.68-05	1.48-04
	3.4656-03	1.51-06	5.99-04	4.78-07	1.90-04	2.39-05	8.01-05
4.0	-1.0983-01	4.19-02	6.11-01	9.07-03	1.32-01	3.36-02	5.50-02
	7.4784-02	9.48-04	6.34-02	2.05-04	1.37-02	2.26-03	4.91-03
	1.8559-02	1.37-04	1.97-02	2.97-05	4.27-03	5.43-04	1.47-03
	8.8094-03	3.97-05	8.66-03	8.60-06	1.87-03	1.96-04	6.22-04
	5.1906-03	1.85-05	4.58-03	4.02-06	9.90-04	8.80-05	3.14-04
	3.4281-03	1.20-05	2.68-03	2.61-06	5.80-04	4.59-05	1.76-04
5.0	-7.2105-02	2.44-02	7.74-01	5.14-03	1.63-01	2.33-02	4.05-02
	5.1722-02	3.23-04	3.07-01	6.80-05	6.48-02	2.17-03	6.32-03
	1.3484-02	4.59-04	2.49-01	9.65-05	5.26-02	6.96-04	5.19-03
	6.6656-03	5.96-04	2.29-01	1.25-04	4.82-02	3.77-04	4.80-03
	4.0531-03	6.35-04	2.19-01	1.33-04	4.62-02	3.19-04	4.62-03
	-3.2148-03	1.98-05	1.54-02	4.17-06	3.24-03	1.39-04	4.35-04

1	2	3	4	5	6	7	8
6.0	-5.7941-02	9.40-03	5.48-01	1.59-03	9.35-02	1.66-02	4.31-02
	4.5041-02	4.82-03	2.33-01	8.20-04	3.96-04	6.27-03	1.83-02
	-2.5910-02	3.37-04	3.39-02	5.73-05	5.76-03	1.17-03	2.57-03
	1.2284-02	5.52-05	1.09-02	9.38-06	1.85-03	3.07-04	7.98-04
	6.2344-03	1.84-05	5.02-03	3.13-06	8.54-04	1.19-04	3.48-04
	3.8594-03	9.72-06	2.76-03	1.65-06	4.70-04	5.72-05	1.79-04
7.0	-5.4801-02	2.01-02	5.59-01	2.65-03	7.37-02	1.82-02	3.35-02
	4.3722-02	1.34-04	9.48-02	1.76-05	1.24-02	2.64-03	5.59-03
	-2.4043-02	6.04-04	6.41-02	7.95-05	8.44-03	1.46-03	3.44-03
	6.1656-03	3.31-05	1.10-02	4.36-06	1.45-03	1.64-04	5.44-04
	3.8281-03	1.46-05	6.19-03	1.93-06	8.15-04	7.91-05	2.90-04
8.0	-4.3410-02	1.74-02	7.03-01	2.22-03	8.96-02	1.59-02	2.91-02
	3.5522-02	5.91-04	2.27-01	7.53-05	2.89-02	1.97-03	4.59-03
	-1.8605-02	8.54-04	2.13-01	1.08-04	2.71-02	1.68-03	3.91-03
	1.0022-02	2.13-04	1.49-01	2.71-05	1.90-02	5.74-04	1.64-03
	5.2156-03	7.67-05	1.23-01	9.77-06	1.56-02	2.75-04	9.13-04
	3.2844-03	2.96-05	1.08-01	3.77-06	1.38-02	1.54-04	5.76-04

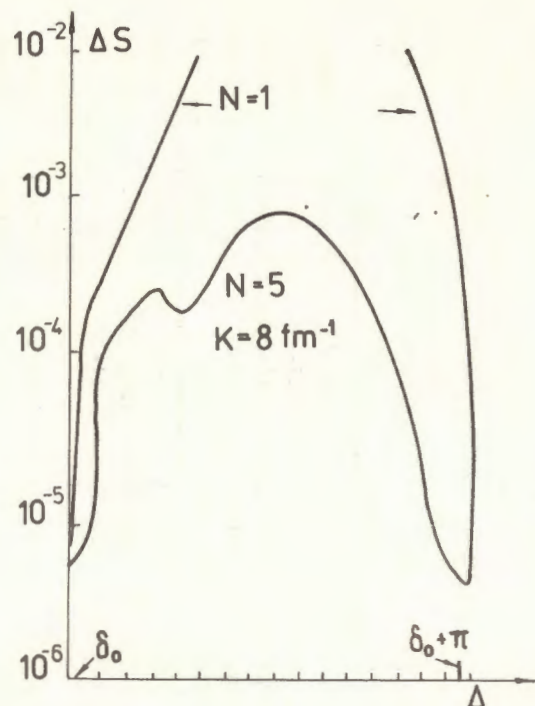


Fig. 3. The  $\Delta$ -dependence of the relative errors  $\Delta S_N$ , calculated according to equation (4.21). Here  $N$  is the number of eigenstates in the expansion, the potential as in fig. 1.

In table 1 we also give the integrated numerical error of the wave function

$$\Delta\Phi = \int_0^a |\Psi^N - \Psi| dz$$

and the maximal numerical error

$$\Delta\Psi = |\Psi^N - \Psi|_{MAX},$$

where  $\Psi^N$  is obtained by taking into account  $N$  terms in the expansion (2.14a).

The convergence of the  $K$ -matrix for  $\Delta = \frac{\pi}{2}$  was investigated for different potentials in ref.<sup>5)</sup>. The other convergence questions, discussed above, seem not to have been investigated earlier. Note that, as seen in table 2, the convergence of the expansion in real Weinberg functions for the Woods-Saxon case is in contrast to what was concluded in ref.<sup>5)</sup>, very fast in a large energy interval ( $0 \leq E \leq 1250$  MeV). Here, with only 2 terms in the expansion, we have  $\Delta S < 1$  percent.

It is interesting to compare the convergence of the real and complex Weinberg expansions. It is seen in table 3 that for the  $S$ -matrix, the expansion in real functions is faster than the other by a factor of  $10^2$  in average. When we compare the expansion in terms of real Weinberg states with the Mittag-Leffler expansion, see table 4, we also see that the former expansion is considerably faster converging than the latter.

All what here is said about the  $S$ -matrix is valid for the expansion of the wave function as well, and we may conclude, that the expansion on terms of real Weinberg functions ( $\Delta = \frac{\pi}{2}$ ) is in general far superior to the other ones.

In the neighbourhood of narrow resonances, this type of expansion must be particularly good; the calculations of Huby and Liu<sup>6)</sup> actually showed, that in some cases, one term is sufficient.

In the general case, as was mentioned above, we still have the possibility of the free choice of  $\Delta$ . In fig. 3 we show, how  $\Delta S$ , for a fixed value of  $K$ , depend on  $\Delta$ . As expected, the convergence of the expansion becomes very fast, when  $\Delta$  approaches the eigenphase  $\delta_0$ ; for  $\Delta = \delta_0$  only one term is needed.



Table 2. The relative errors,  $\Delta S = \left| \frac{S_{\text{exact}} - S}{S_{\text{exact}}} \right|$  in the calculation of the S-matrix by expansion in real Weinberg states ( $N$  indicates the number of terms) for a Woods-Saxon potential;  $\rho = D$ , the potential is that of the text, corresponding to  $^{16}\text{O}$ .

$K (\text{fm}^{-1})$	0.1	1.0	2.0	3.0	4.0	5.0	6.0	7.0	8.0
$N=1$	0.619	1.065	1.265	1.000	0.541	0.362	0.255	0.186	0.139
2	0.079	0.590	0.007	0.004	0.005	0.004	0.006	0.007	0.009
3	0.023	0.012	0.001	0.001	0.001	0.001	0.001	0.003	0.008
4	0.020	0.023	0.006	0.001	0.006	0.005	0.006	0.008	0.010
5	0.019	0.031	0.007	0.004	0.005	0.004	0.005	0.007	0.009
6	0.017	0.004	0.005	0.004	0.003	0.003	0.004	0.006	0.010

Table 3. The relative errors  $\Delta \text{SRW}$  and  $\Delta \text{SCW}$  in the calculation of the S-matrix by expansion in terms of real and complex Weinberg states, respectively ( $N$  is the number of terms) for the rectangular well with the parameters as in table 2.

$N$	$k=0.1 \text{ fm}^{-1}$		$k=1.0 \text{ fm}^{-1}$		$k=5.0 \text{ fm}^{-1}$		$k=8.0 \text{ fm}^{-1}$	
	$\Delta \text{SRW}$	$\Delta \text{SCW}$	$\Delta \text{SRW}$	$\Delta \text{SCW}$	$\Delta \text{SRW}$	$\Delta \text{SCW}$	$\Delta \text{SRW}$	$\Delta \text{SCW}$
1	4.00-05	1.09-04	3.24-04	4.79-03	5.14-03	2.69-03	2.22-03	1.72-03
2	1.58-06	1.10-04	5.08-05	5.21-03	6.80-05	1.08-03	7.53-05	5.86-04
3	1.57-07	1.10-04	6.08-06	5.22-03	9.65-05	1.34-03	1.08-04	5.62-04
4	3.82-07	1.10-04	1.48-07	5.22-03	1.25-04	1.36-03	2.71-05	7.13-04
5	4.33-07	1.10-04	1.55-06	5.22-03	1.33-05	1.36-03	9.77-06	7.28-04
6	4.51-07	1.10-04	1.96-06	5.22-03	4.17-06	1.36-03	3.77-06	7.30-04

Table 4. The relative errors  $\Delta$  SML and  $\Delta$  SRW of the S-matrix calculated by the Mittag-Leffler and real ( $\Delta = \frac{R}{V}$ ) Weinberg expansion, respectively. The potential is a square well of radius 3.26 fm, = 48.72 MeV. The Mittag-Leffler is the optimal expansion (3.18), with 16 terms, in the Weinberg case, 6 terms were used.

	$k = 0.1 \text{ fm}^{-1}$	$k = 1 \text{ fm}^{-1}$	$k = 2 \text{ fm}^{-1}$	$k = 3 \text{ fm}^{-1}$	$k = 4 \text{ fm}^{-1}$
$\Delta$ SML	$\Delta$ SRW	$\Delta$ SML	$\Delta$ SRW	$\Delta$ SML	$\Delta$ SRW
3.06-04	2.12-05	5.96-03	1.12-04	2.92-03	1.73-05
				1.08-03	1.66-04
				1.28-03	4.18-04

	$k = 5 \text{ fm}^{-1}$	$k = 6 \text{ fm}^{-1}$	$k = 7 \text{ fm}^{-1}$	$k = 8 \text{ fm}^{-1}$
$\Delta$ SML	$\Delta$ SRW	$\Delta$ SML	$\Delta$ SRW	$\Delta$ SML
2.13-03	1.37-03	3.25-03	1.29-03	4.70-03
				1.18-03
				6.59-03
				1.08-07

## 5. Conclusion

We have here considered different discrete expansions of continuum single particle wave functions and Green functions, which are solutions of equations with potentials of type, encountered in nuclear physics.

Since, by present day optical model programs, the Schrödinger equation is solved very precisely and fast, these expansions are of little value in connection with the problem of scattering in a potential as such. The usual continuum problems, met in nuclear physics are of a more complicated sort, where residual interactions of different types are important both for elastic and inelastic scattering and for nuclear reactions. The potential scattering wave functions will in such problems only play the role of a first approximation in a perturbation expansion, as in DWBA.

These perturbation methods have a limited region of applicability, and if we think of such processes as  $(\gamma, \rho)$ ,  $(\gamma, n)$ , etc. proceeding at such energies, where the nuclear wave functions are made up of several components, the alternative methods of coupled channels are very tedious.

In such cases, an expansion of the total wave function, including continuous parts (at least in some part of space), in terms of a discrete basis, will be very useful. Such expansions are in use in a wide range of problems, from the expansion of potentials in separable Weinberg terms, used in few body problems, to  $R$ -matrix or NBC expansions, used for heavier nuclei.

In this article, we have compared the convergence properties of some of these expansions, including a new one, our version of the real Weinberg states, only for the case of potential scattering. When residual interactions are taken into account, similar convergence properties must in general exist, as can be argued from the convergence of the Green functions. Only in the case, where a number of eigenvalues lie very near to each other, the admixtures of the corresponding eigenstates, caused by residual interactions are beyond the estimates of perturbation theory. However, this can only concern a limited number of eigenstates, corresponding to different channels (e.g., with different  $\ell$ -values).

The extremely fast convergence of our real Weinberg expansion, in the case when  $\Delta$  approaches the  $\delta$  of the potential



scattering, is of course not expected, when residual interactions are included, still, as mentioned above, this expansion will retain some very nice convergence properties, and in general, both numerical and mathematical facts speak in favour of the real Weinberg (or in some cases the NBC) expansion as being the fastest converging of all.

The practical applicability of expansions does not depend on their convergence properties only. The real Weinberg states may provide the best possible expansion basis, if we want to describe, e.g., elastic scattering with given projectile and target, at a certain energy. If, on the other hand, we are interested in the general solutions of the Schrödinger equation of a given nucleus, the energy dependence of the Weinberg, Kapur-Feierls, and other states of section 4 is a drawback, and an expansion in terms of a fixed basis, like the pole states has great advantages, even if it should turn out, that the number of terms needed is comparatively large.

The authors acknowledge helpful discussions with members of the staffs of the Joint Institute for Nuclear Research and the Niels Bohr Institute.

One of the authors, (J.B.) wants to thank the J.I.N.R. for paying his stay in Dubna during the period in which the work was done, and the Danish Research Council for a grant, covering his travelling costs.

#### Appendix

In this appendix, we shall shortly discuss some different numerical methods, used for obtaining the resonance functions as well as the Weinberg functions, etc.

Here it is convenient to look at the homogeneous Lippman-Schwinger equation

$$G_0(\epsilon) V \psi = \lambda \psi \quad (\text{A.1})$$

(or rather, the radial part of this) satisfied by all these functions, with different  $G_0$  corresponding to the different boundary conditions.

a) The separable representation of the potential was proposed in ref.<sup>5</sup>). Here we get

$$\begin{aligned} V_e(\kappa, \kappa') &= \int_0^\infty j_e(\kappa r) V(r) j_e(\kappa' r) dr \\ &\approx \sum_{i=1}^N V_i j_e(\kappa r_i) j_e(\kappa' r_i) \end{aligned} \quad (\text{A.2})$$

Then (A.1) takes the form

$$\sum_i \left\{ \lambda_{ne}(\epsilon) \delta_{i\kappa} + (V_i V_\kappa)^{1/2} G_{oe}(\kappa_i, \kappa_i, \epsilon) \right\} C_i = 0, \quad (\text{A.3})$$

where

$$C_i = \frac{2}{\pi} V_i^{1/2} \int_0^\infty j_e(\kappa' r_i) \psi_{ne}(\kappa') d\kappa' \quad (\text{A.4})$$

for  $G_{oe}^\pm$  we have

$$G_{oe}^\pm(\kappa_i, \kappa_i, \epsilon) = \frac{2}{\pi} \int_0^\infty d\kappa \frac{j_e(\kappa r_i) j_e(\kappa r_i)}{\epsilon^2 - \kappa^2 \pm i\eta} \quad (\text{A.5})$$

which can be integrated analytically.

The system of equations (A.3) has a symmetric coefficient matrix, which can be diagonalized by simple methods, so the  $\lambda_i$  are easily found. If, instead, we want the resonance values of  $\epsilon$ , for which, again, the determinant of (A.3) is zero, a somewhat complicated calculation is necessary.

Since the separabilization method mentioned above is sufficiently precise for the  $\lambda$  -eigenvalue problem<sup>5)</sup>, the two following methods were mainly used for finding resonances (the  $\epsilon$  -eigenvalue problem). For that case, the method<sup>5)</sup> was used to find a first approximate solution of (A.1). Starting from this, more precise solutions were found by one of the following methods.

b) The finite difference method with stepwise pursuit

Here we approximate the radial Schrödinger equation (2.1a)

$$\varphi_e'' + \left( \kappa^2 - \frac{\epsilon(\epsilon+1)}{r^2} - V(r) \right) \varphi_e = 0 \quad (\text{A.6})$$

with the boundary conditions

$$\varphi(0) = 0 \quad (\text{A.7a})$$

$$\frac{\varphi'(r)}{\varphi(r)} = \beta(\kappa) \quad (\text{A.7b})$$

in terms of finite differences (step length  $h$ ) as respectively

$$D_{n+1} U_{n+1} - C_n U_n + D_{n-1} U_{n-1} = 0 \quad (\text{A.8})$$

and

$$U_0 = 0 \quad (\text{A.9a})$$

$$S_{N+1} U_{N+1} - 2b_h U_N - S_{N-1} U_{N-1} = 0 \quad (\text{A.9b})$$

here

$$U_n = \varphi_e(h \cdot n)$$

$$D_n = 1 - \frac{Q_n h^2}{12}$$

$$C_n = 2 + \frac{5 Q_n h^2}{6}$$

$$S_n = 1 - \frac{Q_n h^2}{6}$$

$$Q_n = V(hn) + \frac{e(e+1)}{(h \cdot n)^2} - K^2$$

which gives an approximation to (A.6), (A.7) with errors  $h^4$ .

This system of difference equations was solved by the method of stepwise pursuit (7,8).

For the quantity

$$A_i = \frac{U_{i-1}}{U_i} \quad (\text{A.10})$$

we get the recursion formula

$$A_{i+1} = \frac{D_{i+1}}{C_i - D_{i-1} A_i} \quad (\text{A.11})$$

Now, the recursion formula is used from both sides, starting with  $A_L$  and  $A_{M+1}$  given by the respective boundary condition (A.9a), (A.9b). The eigenvalue  $K$  is determined by identifying the logarithmic derivatives of the two solutions at some point  $n=M$ . If the  $A_n^L$  obtained by recursion from left and right are called  $A_n^L$  and  $A_n^R$ , respectively, this condition is

$$\frac{S_{M+1} - S_{M-1} A_M^L A_{M+1}^L}{2h \cdot A_{M+1}^L} = \frac{S_{M+1} A_M^R A_{M+1}^R - S_{M-1}}{2h A_{M+1}^R}, \quad (\text{A.12})$$

where  $M+1 = N-M$ .

Table 5. The  $k$ -values of  $6 (\ell = 0)$  resonances of  $^{16}\text{O}$  (the potential of the text, cut at  $R_0 + 10$ -fm calculated with

- The method 17), using 64 points
- The finite difference method, step length 0.01 fm.
- The integral equation method, step length 0.02 fm.

	Rek	Imk	Rek	Imk	Rek	Imk	Rek	Imk	Rek	Imk		
	$\text{fm}^{-1}$	$\text{fm}^{-1}$	$\text{fm}^{-1}$	$\text{fm}^{-1}$	$\text{fm}^{-1}$	$\text{fm}^{-1}$	$\text{fm}^{-1}$	$\text{fm}^{-1}$	$\text{fm}^{-1}$	$\text{fm}^{-1}$		
a	0	1.258	0	-1.257	0	0.440	0.406	-0.738	0.776	-0.669	1.127	-0.638
b	0	1.257	0	-1.256	0	0.438	0.450	-0.728	0.853	-0.673	1.231	-0.671
c	0	1.257	0	-1.256	0	0.438	0.451	-0.728	0.855	-0.672	1.233	-0.670



From this  $K$  is found by iteration, and once it is determined, the solutions are constructed by means of (A.10).

c) Integral equation method

The Lippman-Schwinger equation with  $G_0 = G_0^+$  is equivalent to the Volterra equation.

$$\varphi_e(\kappa, z) = \frac{i}{2} \left\{ \left[ 1 + \frac{1}{\kappa} \int_0^z dz' h_e^+(\kappa z') V(z') \varphi_e(\kappa, z') \right] h_e^-(\kappa z) - \left[ 1 + \frac{1}{\kappa} \int_0^z dz' h_e^-(\kappa z') V(z') \varphi_e(\kappa, z') \right] h_e^+(\kappa z) \right\}. \quad (\text{A.13})$$

Since (A.13) is homogeneous, we may write

$$1 + \frac{1}{\kappa} \int_0^z dz' h_e^+(\kappa z') V(z') \varphi_e(\kappa, z') = 0 \quad (\text{A.14})$$

which may be solved by the methods of ref. 9), using (A.14) as eigenvalue equation.

In table 5 we show some  $K$  values of  $\ell=0$  single particle resonances of  $^{16}\text{O}$  (potential of the text) calculated by the 3 methods described above. The degree of agreement between the very different methods b) and c) indicates the magnitude of the errors.

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