New technique for phase shift analysis: multi-energy solution of inverse scattering problem

S.G. Cooper†, V.I. Kukulin‡, R.S. Mackintosh† and E.V. Kuznetsova††
†Physics Department, The Open University, Milton Keynes, MK7 6AA, U.K.
‡Institute of Nuclear Physics, Moscow State University, Moscow 119899, Russia.
††Institute of Nuclear Research, Russian Academy of Sciences, Moscow 117312, Russia.
(May 28, 1998)

Abstract

We demonstrate a new approach to the analysis of extensive multi-energy data. For the case of d + He, we produce a phase shift analysis covering for the energy range 3 to 11 MeV. The key idea is the use of iterative perturbative data-to-potential inversion which can produce potentials which reproduce the data simultaneously over a range of energies. It thus effectively regularizes the extraction of phase shifts from diverse, incomplete and possibly somewhat contradictory data sets. In doing so, it will provide guidance to experimentalists as to what further measurements should be made. This study is limited to vector spin observables and spin-orbit interactions. We discuss alternative ways in which the theory can be implemented and which provide insight into the ambiguity problems. We compare the extrapolation of these solutions to other energies. Majorana terms are presented for each potential component.

25.45.-z, 25.45.De, 25.10.+s, 24.10.-i, 24.10.Ht

Typeset using REVTEX
A well known problem confronting any phase shift analysis (PSA), both for a single energy and for multiple energies, is the absence of complete sets of experimental data. A complementary problem is the occurrence of apparent inconsistencies between data from different experiments. These problems are particularly acute for projectiles of spin $> \frac{1}{2}$. For example, spin one projectiles require, at each energy, eight or nine independent measurements (cross sections $\sigma(\theta)$, vector $<iT_{11}>$ and tensor $<2q>$ analysing powers, etc.) Since the PSA solutions based on incomplete data will be far from unique, we must find a way to apply constraints. Apart from certain smoothness requirements, it is highly nontrivial to find general restrictions which are convenient to apply within the framework of existing PSA methods.

In this paper we present a new approach to phase shift analysis, PSA. In essence, we describe experimental data, covering a considerable energy range, by a potential which assumes a flexible form that is determined using inversion techniques. Such a potential, while being sufficiently general to fit the data, will nevertheless embody in a very natural way, quite out of the reach of a conventional PSA, physically natural relationships between the many sets of phase shifts. Moreover, the model itself will now reveal any inconsistent data and indicate where new data are required and thereby be a useful source of experimental guidance.

Our present application shows that an integrated picture of $d + ^4\text{He}$ scattering can be obtained from a diverse range of data covering a substantial energy range. The need for such an approach may be seen from the paper of Kuznetsova and Kukulin [1] where a huge amount of experimental data for this reaction, including cross section and vector and tensor analysing powers, are analysed at length by elaborate forms of PSA. Although the authors [1] derived a lot of important information from their PSA (e.g. exact resonance widths, vertex constant etc.) many results are still on a preliminary and qualitative level (e.g. the complex tensor mixing parameters, odd-parity phase shifts). Therefore we believe that the very considerable experimental effort devoted to this system, see [2] and many other papers cited in reference [1], motivates a new approach. Since $d + ^4\text{He}$ is a perfect theoretical test case, the rewards will be physical insight of general relevance to nuclear physics.

In principle the potential searched for should include all necessary components of nuclear interactions, including central (Wigner (W) and Majorana (M)) terms, spin-orbit terms (again, both W and M) and the various possible tensor terms, once more both W and M; all terms may be complex as required. In determining a suitable potential, one can impose constraints and restrictions such as:

- the imposition of an accurate description of higher partial waves (along the lines of OPEP contributions in N-N PSA [3]);
- smooth energy dependence of underlying potentials;
- consistency with established theory, such as double folding models [4];
- incorporation of information concerning bound- and resonant-state energies.

It is possible to carry out a PSA covering many energies by standard searching procedures applied to the parameters of a sufficiently flexible potential model, whether of standard
multi-parameter or model independent (e.g. Fourier-Bessel) form. These procedures generally entail computationally expensive and highly non-linear multi-parameter fitting, often leading to many local minima [5]. The approach we present here, the IP inversion procedure [6–10], avoids these problems to a considerable extent. Two of the advantages of IP over other inversion methods are particularly relevant. The first is that the exactness of the inversion may be controlled, so that noisy, incomplete or even partly erroneous data can be fitted with (one-channel or multi-channel) potentials which do not contain spurious oscillatory features. The second advantage is its virtually unlimited generalizability. The method is also fast and so enables a thorough exploration of ambiguity problems which are not a matter of shallow valley floors in parameter hyper-space, but appear in the form of apparently disconnected minima.

In the present case we apply the procedure to \( S = 1 \) projectiles, although for clarity we suppress spin-related subscripts. The method involves the following three key elements:

(i) Expansion of components of the potential (central (c), spin-orbit (s-o), tensor (t), etc.) in a suitable basis. For potential component \( k = c, s-o, t \ldots \)

\[
\mathbf{V}^{(k)} = \mathbf{V}_0^{(k)} + \sum_j C_j^{(k)} \phi_j^{(k)}(r)
\]

where \( C_j^{(k)} \) are coefficients to be determined, \( \phi_j^{(k)}(r) \) are the basis functions and \( \mathbf{V}_0^{(k)} \) is the starting potential. Note that this expansion applies to both real and imaginary components and that the notation \( \phi_j^{(k)}(r) \) embodies the possibility that it might be appropriate for different components of the potential to be expanded in different bases. In particular, real and imaginary terms, or central and spin-orbit terms, might well require different bases.

(ii) The linear response of the complex \( S \)-matrix \( S_l \) to small changes \( \Delta V(r) \) in the potential:

\[
\Delta S_l = -\frac{im}{\hbar^2k} \int_0^\infty (\psi_l(r))^2 \Delta V(r) dr
\]

with \( S_l \) defined in terms of the asymptotic form of the regular radial wave function as \( \psi_l(r) \rightarrow I_l(r) - S_l O_l(r) \) where \( I_l \) and \( O_l \) are incoming and outgoing Coulomb wave functions of Ref. [4]. The formulation [7,8] in terms of \( \delta_l \), where \( K_l = \tan \delta_l \), is exactly equivalent. Note that the energy \( E_k \) is implicit in these equations and, for simplicity, we have labelled the channels only by the orbital angular momentum \( l \) although we do include spin in our calculations. Equation 2 can be recast as [6,9]:

\[
\frac{\partial S_l}{\partial C_j} = -\frac{im}{\hbar^2k} \int_0^\infty (\psi_l(r))^2 \phi_j(r) dr
\]

where any required superscript \( (k) \), labelling the potential component, is implicit.

(iii) To establish an overall linearization, we next linearize the \( \chi^2 \) function:

\[
\chi^2 = \sum_{k=1}^{N} \left( \frac{\sigma_k - \sigma_{k}^{in}}{\Delta \sigma_k^{in}} \right)^2 + \sum_{n=1}^{M} \sum_{k=1}^{N} \left( \frac{P_{kn} - P_{kn}^{in}}{\Delta P_{kn}^{in}} \right)^2
\]

where \( \sigma_k^{in} \) and \( P_{kn}^{in} \) are the input experimental values of cross sections and analyzing powers of type \( n \) respectively. Since we are fitting data for many energies at once, the index \( k \)
indicates the energy as well as angle. To optimise the potential, we require the derivatives of $\chi^2$ with respect to the potential components $C_j^{(k)}$ in Equation 1

$$\frac{\partial \chi^2}{\partial C_i} = 2 \sum_{k,l} \frac{\sigma_k - \sigma_k^{in}}{(\Delta \sigma_k^{in})^2} \frac{\partial \sigma_k}{\partial S_l(E_k)} \frac{\partial S_l(E_k)}{\partial C_i} + 2 \sum_{n,k,l} \frac{P_{kn} - P_{kn}^{in}}{(\Delta P_{kn}^{in})^2} \frac{\partial P_{kn}}{\partial S_l(E_k)} \frac{\partial S_l(E_k)}{\partial C_i}.$$  (5)

We also assume that $S_l$ is locally linear about some current point $\{C_j^{(p)}\}$:

$$S_l(C_j) = S_l(C_j^{(p)}) + \sum_j \frac{\partial S_l}{\partial C_j} \Delta C_j,$$  (6)

which applies at each iterative step $p = 0, 1, 2, \ldots$ and the correction (to be determined) for the $j$-th amplitude is $\Delta C_j = C_j - C_j^{(p)}$. We now solve the linear equations which follow [8], by way of Equation 5, from demanding that $\chi^2$ be locally stationary with respect to variations in the potential coefficients $C_i$. This is straightforward for any reasonable number of them and yields corrected values $C_j^{(p)}$ [8,10]. We then iterate the whole procedure, with wave-functions $\psi_l$ in Equation 3 calculated using current values of the coefficients, until convergence is reached. This algorithm almost always converges very rapidly [8,10], in general diverging only when highly inconsistent or erroneous data have been used or when the iterative process involves a very unsuitable starting point.

We have thus reduced the whole multi-energy inversion to the solution of simultaneous equations at a series of iterative steps. To demonstrate the effectiveness of this approach, we now present the results of a multi-energy PSA for the $d + ^4$He system. For this initial study, we have selected a small subset of the experimental data tabulated in [1], in particular the data of Jenny $et$ $al$ [2] and that of [11,12]. At this stage, we have fitted only the cross sections and vector analysing powers and correspondingly limited ourselves to the following potential components: Wigner central; Majorana central; Wigner spin-orbit; Majorana spin-orbit. All terms are complex so that there are eight components to be determined. The neglect of the various complex tensor components is justified because these seem to have little effect on any data other than the tensor analysing powers. It is well known [13,14] that tensor interactions in the $d + ^4$He system play a moderate role, mainly influencing the $3S_1 - 3D_1$ and $3P_2 - 3F_2$ mixing parameters which are not significant here. Nevertheless, our approach can be generalized to yield tensor interactions. The full PSA, including all off-diagonal terms, will be presented in a subsequent publication.

In order to get some understanding of the ambiguity problems, we consider here two extreme approaches to the fitting process which we label A and B. The question of the meaningfulness of the potentials that are found we leave to later publications.

Approach A begins the iterative procedure with a starting potential reflecting very little a priori information concerning the potential and consists of two components only: simple real and imaginary central Wigner terms of Gaussian form. The data is fitted in stages, adding a further potential component at each step with basis dimensions restricted to two or three Gaussian functions. Generally convergence results from two or three inversion iterations at each stage. By applying a criterion of visual smoothness, an optimum solution was found, ‘potential A’, corresponding to $\chi^2/F = 18.7$. Fits giving a lower $\chi^2/F$ are possible with a
larger basis, but the corresponding $|S|$ also show a significant unitarity breaking for certain $l,j$.

*Approach B* starts the iterative procedure with a potential derived by inversion [15] of $S_{lj}$ from the multi-configuration RGM calculations of Kanada et al [16] which include S-wave deuteron breakup. This approach gave ‘potential B’ with $\chi^2/F = 5.84$ but is accompanied by a significant breaking of unitarity in the S wave. (The results are described in detail in Ref. [22].)

In both approaches energy dependence is included only in the imaginary components. The procedure used follows Ref. [19], which applies for shape invariant energy dependent potentials. Since the inelastic threshold is at $E_{th} = 3.3$ MeV, we expect the imaginary components to increase rapidly as the energy rises above $E_{th}$ and so we assume that all parts of the imaginary potential increase linearly with $(E - E_{th})$. In fact, the results are insensitive to this energy dependence. Both the detailed form of the imaginary potentials and the imaginary phase shifts are less well determined than the corresponding real quantities and qualitative features of the data can be reproduced with a real potential alone.

In Figure 1 we display, for representative energies over the complete energy range of 3 – 11.5 MeV, typical fits to cross sections [12] and in Figure 2, analyzing powers [11]. Both $\sigma(\theta)$ and $<iT_{11}(\theta)>$ are very well fitted over the entire energy range. Closely compatible fits to the data of Ref. [2] were found, both visually and in the values of $\chi^2$, and will be discussed in a more detailed account. All the quoted $\chi^2/F$ values apply to the fit over the full energy range, but are only relative since the tabulated data did not include all the sources of error discussed in the original papers. Furthermore, theoretical calculations suggest that although the contribution of the mixing parameters is almost negligible for the cross-section, a more noticeable contribution is found for the fit to the $<iT_{11}(\theta)>$ data.

The bound state energy of the $^4$He – d system, which can be identified as the ground state energy of $^6$Li in the $^4$He – d channel, is not included in these inversions. Potential A gives $E_B = -2.26$ MeV ($E_B^{\text{expt}} = -1.472$ MeV). Note that this energy is extremely sensitive to the form of the potentials and to the energy dependence of the d – $^4$He $^3$S$_1$ phase shifts [17].

In Figure 3 we present the real parts of potentials A only, since this solution is clearly preferable from the physical point of view. However the known ambiguity problems suggest this potential is almost certainly not unique. Within either approach, A or B, certain potential components are more reliably determined than others, the real central Wigner term being the best determined. Its volume integral is consistent with global potentials and also with volume integrals of the corresponding potential derived by $S$-matrix to potential inversion for the theoretical $S_l$ of resonating group model (RGM) calculations [8,15,17,18].

The phase shifts corresponding to the solution A for $l \leq 4$ are displayed in Figure 4 for an energy range of 0 to 15 MeV laboratory energy, i.e. extrapolating outside the range of the data. This figure also includes the results of previous PSA data, [2]. The really difficult problem for all previous (standard) PSAs was to achieve a low energy description of odd partial waves (i.e. $^3P_j$ with $j = 0, 1, 2$ and $^3F_j$ with $j = 2, 3, 4$), due to the weak sensitivity of cross sections and analysing powers to the odd partial waves [1]. Thus, by fitting all significant partial waves independently in the course of a standard PSA [1,2], a range of solutions are possible which are consistent with the data. The resulting phase shifts have very large error bars. In the present method for phase shift analysis a further restriction is applied by demanding a smooth underlying potential and therefore the approach should
lead, in principle, to much more reliable and accurate values for all phase shifts than found in previous PSAs [1,2].

The comparison in Fig. 4 of our new PSA solution with previous results, [2], shows that the agreement for even partial waves is quite close while there is less agreement for odd partial waves. A possible reason for this is our neglect of tensor forces. Reliable knowledge of the odd partial wave phase shifts is crucially important [18,20], since the nature of the deuteron – nucleus interaction, particularly for d + 4He, is different for even and odd partial waves. The even parity d + 4He interaction is determined by an intermediate state in which two nucleons in the deuteron occupy two (1p)-orbitals beyond the 4He core. However, for odd parity, the equivalent two outer nucleons occupy non-overlapping 1p–2s or 1p–2d orbits (designating orbits Ni, with N the number of oscillator quanta). Thus, since the N–N interaction is short ranged compared to the range of d – 4He interaction, the contribution of virtual breakup should be higher for odd than for even partial waves and the sensitivity to the N + α interaction should also be higher. Due to this feature of the d + 4He interaction, the p- and f-wave phase shifts have been shown [20] to give a strong test of supersymmetrical aspects of composite particle interactions and the structure of tensor interactions of deuterons. A further step now is to include in our potential terms which have never previously been considered for nucleus-nucleus interactions: complex Majorana tensor forces. Preliminary results [21] show that the Majorana tensor force is approximately as strong as the Wigner tensor force.

In summary: we have proposed a linearized iterative approach for direct inversion from multi-energy data to potentials specifically as a new approach to PSA. It is computationally efficient and avoids many drawbacks and instabilities of conventional PSAs, especially in cases of projectile of spin 1 or greater when one generally has an incomplete data set with data at many relevant energies absent or having large error bars. As well as correct phase shifts, the potential itself is of great interest since it can be used as input for other calculations and can also be compared with potentials found by double folding procedures or by inversion from S_i obtained from RGM and other theoretical models.

ACKNOWLEDGEMENTS

The authors are very grateful to V.N. Pomerantsev for many fruitful discussions on the topics discussed here. One of the authors, (V.I.K.) is grateful to Willi Gruebler for supplying him the full tables of experimental data of the Zürich group. We are also most grateful to the UK EPSRC for grant GR/H00895 supporting S.G. Cooper, the Russian Foundation for Basic Research (grant 97-02-17265) for financial assistance and to the Royal society (UK) for supporting a visit by V.I. Kukulin to England.
REFERENCES


FIGURES

FIG. 1. For deuterons scattering from $^4$He, fits to differential cross sections of Senhouse and Tombrello at selected energies. The solid line is the fit for potential A, the dashed line for potential B.

FIG. 2. For deuterons scattering from $^4$He, fits to vector analysing power data of Gruebler et al at selected energies. The solid line is the fit for potential A, the dashed line for potential B.

FIG. 3. The real parts of potential A (dashed). From top, the Wigner central and spin-orbit, then the Majorana central and spin-orbit.

FIG. 4. The real phase shifts for fit A (solid line) compared with the results of the phase shift analysis of Jenny et al (filled circles).