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

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Abstract

We demonstrate a new approach to the analysis of extensive multi-energy data. For the case of d + ⁴He, we produce a phase shift analysis covering for the energy range 3 to 11 MeV. The key idea is the use of a new technique for data-to-potential inversion which yields 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
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 $> 1/2$. For example, spin one projectiles require, at each energy, eight or nine independent measurements (cross sections $\sigma(\theta)$, vector $i(T_{11}(\theta))$ and tensor $T_{2q}$ 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, the idea is to find a single multi-component potential to describe the experimental data over the energy range in question. This is made possible by a recently developed direct data-to-potential inversion technique, the generalized iterative perturbative method, hereafter GIP, which we describe below. GIP is a generalization of the established IP $S$-matrix-to-potential inversion method [1]. It enables data for many energies to be fitted with great computational efficiency by a single energy dependent potential that is as flexible as required. A PSA based on a potential, unlike conventional PSAs, leads in a natural way to sets of phase shifts bearing physically reasonable relationships between the different partial waves. 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. The GIP potential will have a small energy dependence which, unlike the rapid energy dependence of the phase shifts, can be compared with the energy dependence predicted by theory.

We demonstrate our approach by applying the method to $d + ^4$He and will show that an integrated picture of $d + ^4$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 Ref. [6] 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. The methods used are described by Krasnopolsky et al. [7]. Although the authors of [8] derived much 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 [8] and many other papers cited in reference [9], motivates a new approach. Since $d + ^4$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 such as: conformity to known behaviour of higher partial waves (as in, e.g. [10]); smooth energy dependence of underlying potentials; consistency with established theories; reproduction of bound- and resonant-state energies.

In principle it is possible to find a potential fitting data at many energies by applying standard searching procedures to the parameters of a sufficiently flexible potential model, whether of standard multi-parameter or model independent form (e.g. the so-called Fourier-
To do this generally entails computationally expensive and highly non-linear multi-parameter fitting, often leading to many local minima [10]. The GIP procedure for direct data-to-potential inversion solves many of these problems. The advantages of IP over other methods for $S$-matrix-to-potential inversion apply here too and are particularly relevant. The first advantage is the power to control the exactness of the inversion so that noisy, incomplete or even partly erroneous data can be fitted with (one-channel or multi-channel) potentials which do not have spurious oscillatory features. The second advantage is its virtually unlimited generalizability. Here we illustrate this feature by including in our analysis the four Majorana components, normally omitted in optical model fits. A further feature of PSA using the GIP method is its speed and simplicity of application enabling a thorough exploration of ambiguities. These ambiguities are \textit{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 $k = c, s-o, t, \ldots$

\[
V^{(k)} = V_0^{(k)} + \sum_j C_j^{(k)} \phi_j^{(k)}(r) \tag{1}
\]

where $C_j^{(k)}$ are coefficients to be determined, $\phi_j^{(k)}(r)$ are the basis functions and $V_0^{(k)}$ 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, or the Majorana 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:

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

with $S_l$ defined in terms of the asymptotic form of the regular radial wave function as $\psi_l(r) \rightarrow I_l(r) - O_l(r)\Delta V(r)$ where $I_l$ and $O_l$ are incoming and outgoing Coulomb wave functions of Ref. [11]. The formulation [3,1] 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 [2,4]:

\[
\frac{\partial S_l}{\partial C_j} = -\frac{i m}{\hbar^2 k} \int_0^\infty (\psi_l(r))^2 \phi_j(r) dr \tag{3}
\]

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

(iii) The $\chi^2$ function is defined from:

\[
\chi^2 = \sum_{k=1}^N \left( \sigma_k - \sigma_k^{in} \right)^2 + \sum_n \sum_{k=1}^M \left( \frac{P_{kn} - P_{kn}^{in}}{\Delta P_{kn}^{in}} \right)^2 \tag{4}
\]
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. The data normalising factors can be introduced as an additional contribution to Equation 4.

We must now expand $\chi^2$ in terms of the $C_j^{(k)}$. To do this we first linearize the theoretical cross sections and analyzing powers, by expanding $\sigma_k$ (and $P_{kn}$) about some current point $\{C_j^{(k)}(p)\}$:

$$\sigma_k = \sigma_k(C_j^{(k)}(p)) + \sum_{j,l} \left( \frac{\partial \sigma_k}{\partial S_l(E_k)} \frac{\partial S_l(E_k)}{\partial C_j^{(k)}} \right) C_j^{(k)}(p) \Delta C_j^{(k)}, \quad (5)$$

which applies at each iterative step $p = 0, 1, 2, \ldots$ and the correction (to be determined) for the $j$-th amplitude is $\Delta C_j^{(k)} = C_j^{(k)} - C_j^{(k)}(p)$. Equivalent relations are applied for the $P_{kn}$.

Linear equations result from demanding that $\chi^2$ be locally stationary with respect to variations in the potential coefficients $C_j^{(k)}$, i.e. the derivatives of $\chi^2$ with respect to the potential components $C_j^{(k)}$ must vanish. Solving these linear equations is straightforward for any reasonable number of them and yields corrected values $C_j^{(k)}(p)$ [8,10]. We then iterate the whole procedure, with wave-functions $\psi_l$ in Equation 3 calculated using the corrected potentials from Equation 1, 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.

Multi-energy inversion is thus reduced to the solution of simultaneous equations at a series of iterative steps. To show how effective this is, we present the results of a multi-energy PSA for the $d + ^4He$ system. For this initial study, we have selected a small subset of the experimental data tabulated in [6], in particular the data of Jenny et al [8] and that of [12,13]. 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 their primary effect is on the tensor analysing powers. It is well known [4,13] that tensor interactions in the $d + ^4He$ system play a moderate role, mainly influencing the $^3S_1 - ^3D_1$ and $^3P_2 - ^3F_2$ mixing parameters which are not significant here. The generalisation of GIP to yield tensor interactions is under development and we expect a full PSA, including all off-diagonal terms, to be presented in due course. Data renormalization was not considered here since its effect is small compared to neglect of the tensor force, particularly for the data sets fitted here [1,7].

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 $l, j$. This case involves about 20 independent parameters.

**Approach B** starts the iterative procedure with a potential derived by inversion of $S_{lj}$ from the multi-configuration RGM calculations of Kanada et al. 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. [18].)

In both approaches energy dependence is included only in the imaginary components. The procedure used follows Ref. [21], which applies for shape invariant energy dependent potentials. Since the inelastic threshold is at $E_{\text{th}} = 3.3$ MeV, we expect the imaginary components to increase rapidly as the energy rises above $E_{\text{th}}$ and so we assume that all parts of the imaginary potential increase linearly with $(E - E_{\text{th}})$. 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 and in Figure 2, analyzing powers. Both $\sigma(\theta)$ and $i\langle T_{11}(\theta) \rangle$ are very well fitted over the entire energy range. Closely compatible fits to the data of Ref. [8] were found, both visually and in the values of $\chi^2$. 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. We have found that although the contribution of the mixing parameters to the cross-section is almost negligible, there is a more noticeable effect on the fit to $i\langle T_{11}(\theta) \rangle$.

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 ($E_B^{\text{exp}} = -1.472$ MeV). Note that this energy is extremely sensitive to the form of the potentials and to the energy dependence of the d – $^4$He $^3S_1$ phase shifts.

In Figure 3 we present the real parts of potentials A. 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.

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 a previous analysis. 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. Thus, by fitting all significant partial waves independently in the course of a standard PSA, a range of solutions are possible which are consistent with the data. The resulting odd-parity 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 [6,8].

The comparison in Fig. 4 of our new PSA solution with previous results, shows that the agreement for even partial waves is quite close while there is less agreement for odd partial waves. This is probably due our neglect of tensor forces. Reliable knowledge of the odd partial wave phase shifts is crucially important [20,22], since the nature of the deuteron – nucleus interaction, particularly for $d + ^4\text{He}$, is different for even and odd partial waves. The even parity $d + ^4\text{He}$ interaction is determined by an intermediate state in which two nucleons in the incident deuteron occupy two (1p)-orbitals beyond the $^4\text{He}$ core. However, for odd parity, the two outer nucleons occupy non-overlapping 1p–2s or 1p–2d orbits (designating orbits $Nl$, with $N$ the number of oscillator quanta). Thus, since the N–N interaction is short ranged compared to the range of $d – ^4\text{He}$ interaction, the contribution of virtual breakup should be higher for odd than for even partial waves and the sensitivity to the $N + \alpha$ interaction should also be higher. Due to this feature of the $d + ^4\text{He}$ interaction, the p- and f-wave phase shifts have been shown [22] 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 [23] show that the Majorana tensor force is approximately as strong as the Wigner tensor force.

In summary: we have demonstrated a new approach to PSA based on a linearized iterative approach to direct inversion from multi-energy data to potentials. The example presented, approach A, involved far fewer parameters than a conventional PSA (about a hundred for this case). The new method 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 $S_l$ obtained from RGM and other theoretical models.

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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. 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 a conventional phase shift analysis (filled circles).
\[\sigma(\alpha)\]

\[\theta \text{ (deg.)}\]

- $E = 2.94$
- $E = 4.73$
- $E = 5.96$
- $E = 7.48$
- $E = 9.48$
- $E = 11.5$
