Quantal inversion of the cross section for the elastic scattering of 200 MeV protons from ^{12}C

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Fixed energy quantal inverse scattering theory has been used to analyze the differential cross section from the elastic scattering of 200 MeV protons from ^{12}C. Ambiguities in obtaining the scattering function from the differential cross section are discussed and we illustrate by means of example that not all scattering functions lead to physically reasonable potentials.

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I. INTRODUCTION

Direct procedures are the most common ones used to analyze (fixed energy elastic) scattering data that one obtains from particle beam experiments, whether those experiments are of nuclear, atomic, or molecular systems. In the main those direct procedures are purely phenomenological with a parametric form chosen *a priori* to be the (central, local) interaction between the colliding entities. Increasingly, however, those interactions (or at least the real parts of them) have been defined by folding some underlying pairwise microscopic interaction with the density distributions of the colliding quantal systems. Whichever approach to the direct procedure is used, there is a set of parameters that identify the scheme; the values of which are adjusted to give a best fit to the measured data. That best fit is specified, usually, by finding a minimum chi square (χ^2) fit to the data from variations in the fixed parameter space. A better measure though is to consider the chi square per degree of freedom (χ^2/F) where the number of degrees of freedom is simply the difference between the number of data points used in the search and the number of parameters being varied.

Inverse scattering methods form a complementary procedural class with which to analyze the same data. With inverse methods, the interaction between the colliding pairs is extracted from the data without *a priori* assumptions as to the form of the interaction, although the specific inversion method used to obtain them usually defines the broad class of potentials to which they belong. The underlying dynamical equation of motion is assumed to be known however, and in the case of interest that is the Schrödinger equation. But there is always a question of uniqueness as the experimental elastic differential cross-section data at a given energy only determine the scattering function at the physical (integer) values of the angular momentum and, as we shall see in this paper, not necessarily uniquely. Very different fits with similar statistical significance can be obtained. Then only after interpolation has been made on the chosen scattering function for all pertinent real values of angular momentum, is the corresponding potential obtained by inversion specified uniquely.

Of all of the methods of inversion of fixed energy (cross-section) scattering data, those predicated upon a rational function representation of the underlying scattering (S) function arguably are the most useful. Those forms for the S function facilitate solution of the inverse problem for the Schrödinger equation either by a semiclassical, WKB, procedure (given that conditions are appropriate for use of such an approximation) or by fully quantal schemes. Of the latter, the Lipperheide-Fiedeldey (LF) type [1] are of particular interest, and they have been used quite extensively in recent years to analyze the elastic scattering cross sections from the scattering of two nuclei. The attendant fits to measured data in those cases were usually an order of magnitude better than any obtained by direct methods of analyses [2].

Herein we consider the inversion, using a fully quantal method, of the differential cross-section data [3] from the elastic scattering of 200 MeV protons from ^{12}C. At present, the LF methods of data inversion do not allow for a spin-orbit interaction and its role, however minor, in defining cross sections. But it is of interest to study this reaction with our inversion methods to ensure that the fully quantal procedures can be used in such cases of a very light projectile on a light ion. Also the 200 MeV data are reasonably, but not supremely, well described by direct means, whether they involve a purely phenomenological [3] or fully microscopic folding model [4,5] defined optical potential. Of even greater interest, however, is that the data are quite extensive both in number of measured values and in range of momentum transfer. Furthermore, the data set has small nonstatistical errors. As a consequence, a sensible error analysis of the potentials given by inversion becomes feasible, enabling us to place confidence bounds on that potential. This has been the case in the past with electron-atom data [6].

Following a brief review of the inverse scattering theory and of the LF methods that we have used in our analysis, the results of the calculations are discussed in Sec. III.

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II. ELEMENTS OF FIXED ENERGY INVERSE SCATTERING THEORY

Solutions of the Schrödinger equation with a central, local interaction describing the collision of two quantal systems, link to measured data via scattering amplitudes that one extracts from the asymptotic forms of those solutions. In the center of mass frame, the scattering amplitude is related to the differential cross section by

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 \ . \tag{1}$$

In the partial wave treatment of the scattering, the scattering amplitude can be defined in terms of an S function by

$$f(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)[S(l)-1]P_l(\theta) \ , \tag{2}$$

where $S(l)$ are the values of the S function, $S(\lambda)$, for the (positive) integer values of the angular momentum variable λ ($l = \lambda - \frac{1}{2}$). That S function relates to the phase shift function, $\delta(\lambda)$, by

$$S(\lambda) = \exp[2i\delta(\lambda)] \ , \tag{3}$$

and is usually displayed in modulus and phase form, viz.

$$S(\lambda) = |S(\lambda)| \exp[2i\mathcal{R}(\delta(\lambda))] \ . \tag{4}$$

It also relates to the classical deflection function, a function that is a reflection of the physical processes involved in the scattering, by

$$\Theta(\lambda) = 2\frac{d\delta(\lambda)}{d\lambda} = \frac{d\ln[S(\lambda)]}{d\lambda} \ . \tag{5}$$

Usually $S(\lambda = l + \frac{1}{2})$ is determined from the differential cross section by means of a least squares fitting procedure. It is important to notice that not only is this procedure ambiguous, and that will be clearly illustrated in this paper, but also the measured data are only sensitive to that S function at the integer values of l.

The inverse scattering problem for fixed energy scattering then resolves to the following: *Given the S function at a particular energy and as a function of the angular momentum, find the central, local potential which reproduces that S function.* But the S function must be defined at all (continuous) values of the angular momentum variable, $\lambda \geq 0$, before the potential obtained by inversion is uniquely defined. Thus to proceed with inversion of the Schrödinger equation for fixed energy scattering, one must interpolate and extrapolate upon the set of S-function values, however they are obtained by fits to measured data.

There are several methods of solution of the quantal fixed energy inverse scattering problems. Herein we will consider application of a fully quantal method based upon a Lipperheide-Fiedeldey scheme, details of which have been published [1]. In the simplest of those schemes, one assumes that the fixed energy S function for scattering can be represented by a complex, rational function form:

$$S(\lambda) = S_0(\lambda) \prod_{n=1}^{N} \frac{\lambda^2 - \beta_n^2}{\lambda^2 - \alpha_n^2} \ . \tag{6}$$

Then the total scattering potential [$V(r) = V_N(r)$] can be obtained by iteration as

$$V_n(r) = V_{n-1}(r) + \Delta^{(n)}(r) \ , \tag{7}$$

where, with V_0 being the potential associated with the reference S function $S_0(\lambda)$ and the increment function for each additional pole-zero pair of the N set defining the S function is given in terms of the Jost solutions from the preceding iterate of the potential by

$$\Delta^{(n)}(r) = \frac{2i}{r}(\beta_n^2 - \alpha_n^2)\ \frac{d}{dr}\left(\frac{r}{L_{\beta_n}^{(-)}(r) + L_{\alpha_n}^{(+)}(r)}\right) \ . \tag{8}$$

Therein $L_\lambda^{(\pm)}(r)$ are logarithmic derivatives,

$$L_\lambda^{(\pm)}(r) = \pm i \left(\frac{\frac{d}{dr} f_\lambda^{(\pm)}(r)}{f_\lambda^{(\pm)}(r)}\right) \ , \tag{9}$$

with $f_\lambda^{(\pm)}(r)$ being the Jost solutions of the potential [$V_{n-1}(r)$] that asymptote as $e^{\mp ikr}$, respectively. Extension to a class of nonrational S functions has also been achieved [1] and a "mixed" method [7], which employs a product of rational and nonrational S functions, has been used in applications as well [2].

III. RESULTS AND DISCUSSION

The final check on any fixed energy inversion study of nuclear scattering is the comparison of cross sections obtained from the phase shifts one gets by using the potentials derived by inversion, with the data that was used in the first instance to find the input (S function) to that

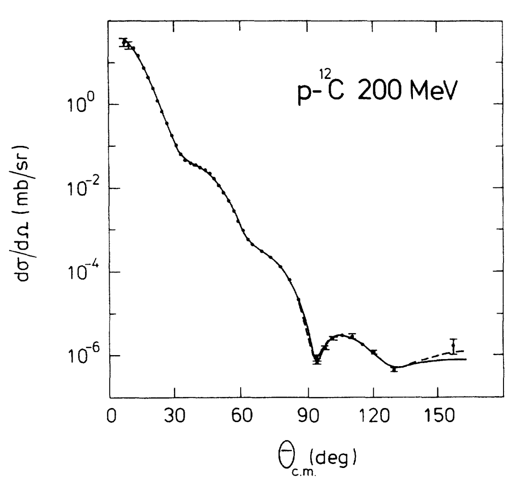

FIG. 1. The differential cross-section data and two fits to them that result by using potentials obtained by inversion of that data in the Schrödinger equation.

inversion process. In the present case the 200 MeV p-^{12}C cross sections so obtained are compared with the data [3] in Fig. 1. There are two results shown and both are in extremely good agreement with the measured values. Specifically, those fits to data have χ^2/F values of 1.006 and 1.018 for the solid and dashed curves, respectively, when a reference S function of the form

$$S_0(\lambda) = e^{i\eta \ \ln[\lambda^2+\lambda_c^2]} \ , \tag{10}$$

where η is the Sommerfeld parameter, was used. These results are of similar statistical significance but have been obtained by using quite different S functions, and concommitantly, phase shift and deflection functions. The total S and deflection functions (Coulomb scattering has been included) are shown in Fig. 2. The S functions are displayed in modulus and phase while the deflection functions are given in real and imaginary parts. Both S functions were obtained assuming a rational form for them and varying the parameters therein to fit the cross-section data directly. Model forms for the "experimental" S function, such as used in past studies of heavy ion collisions [2], have not been considered. The two results were found by using quite different starting conditions in a search upon the (complex) values of a set of five pole-zero pairs $\{\alpha_n, \beta_n\}$ that define the rational scattering function. In the first search, the initial set of parameter values were chosen arbitrarily (we denote the parameter set so found after minimization as set 1). The second set (set 2), on the other hand, was obtained by starting with a set of pole-zero parameter values that map the S function obtained from using the best phenomenological optical model potential [3] in the Schrödinger equation. Those values were then varied to obtain an improved fit to the data and the final results are listed in Tables I and II. The reference S function used in both cases was that of shifted point Coulomb form with parameter λ_c having the value 3η. The pole-zero values are given to 10 decimal places to stress that extreme accuracy need be carried so that the rational function will give the S-function values with the many significant digits that are required to so accurately fit the cross-section data.

It is evident from Fig. 2 that the two approaches in defining the S function have led to quite different minima and they provide a striking illustration of the ambiguity in the relationship between the differential cross section and the scattering function. The S and deflection functions we find with the parameters of set 1 are far more structured and have significant values (in terms of effect in fitting the cross-section data) for a very large range of l values. It is not surprising to find therefore, that, when used in the appropriate fully quantal inversion scheme of LF type, these two parameter sets yield markedly different complex, local effective interactions. The real and imaginary components of those potentials obtained by inversion are compared in Fig. 3 with the best phenomenological (central) one [3], and designated as a double Woods-Saxon (DWS) in that reference. The inversion result obtained from set 2 is displayed therein by the solid curves, the result obtained from set 1 is shown by the dashed curves and the DWS phenomenological interaction is represented by the dot-dashed lines. Clearly the phenomenological potential has an imaginary part very similar to that we find with our (initially) "constrained" search result (set 2). The real part of both inversion potentials, however, are far more attractive overall than the phenomenological one. But it must be remembered that the phenomenological interaction does not give a very good fit to the cross-section data. Both potentials obtained by inversion yield excellent fits. The parameters of set 1 are quite unphysical however. They yield a very strongly absorptive potential and imply extreme long range effects; the consequence of very many (too many) partial waves being required to explain the data. Our preferred result is set 2 which was based upon a starting optical model scattering function. It is much more refractive than the other, and as such, it is more like results one finds by folding realistic NN g matrices with nuclear densities to define a (microscopic) optical model potential [4,5] than are those obtained with current phenomenological forms. As stated, the potential corresponding to set 1 we find to be quite unrealistic; being extremely long ranged and excessively absorptive. But it is a potential which when used in solving

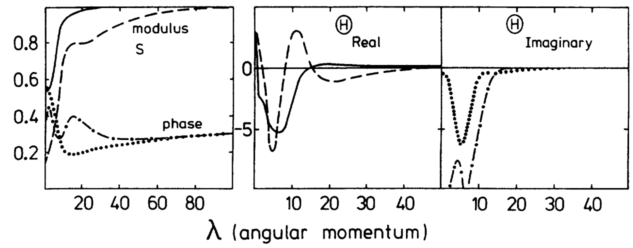

FIG. 2. The S and deflection functions defined by the two sets of rational form parameters that were found by fitting the differential cross-section data. The curves are identified in the text.

TABLE I. The rational function parameters, set 1, that gave the fit to the 200 MeV p-^{12}C cross-section data with χ^2/F of 1.006.

	α_n		β_n	
	Real	Imaginary	Real	Imaginary
1	10.2446786946	-5.9807367075	1.5796064650	3.6195027016
2	26.5439785204	-42.5669791285	0.4686569859	2.6866969870
3	2.6881915849	-3.1400601804	-4.4316628648	3.2510333349
4	-2.6559990678	-2.7192349896	-12.4204548530	11.1907290021
5	-2.8946159284	-16.0423535307	-23.2285401587	43.0799819080

TABLE II. The rational function parameters, set 2, that gave the fit to the 200 MeV p-^{12}C cross-section data with χ^2/F of 1.018.

	α_n		β_n	
	Real	Imaginary	Real	Imaginary
1	-0.0548404233	-1.2599738423	-0.1326287045	1.2346281412
2	-6.1751408446	-9.0868456370	-3.7452076971	3.8048412982
3	-7.7899061381	-4.2929187247	-10.3231568381	7.6141819546
4	10.6813616392	-8.0296693873	4.0784716287	7.7628740770
5	3.2755483843	-5.1539508135	7.8586850920	5.9266030850

the Schrödinger equation, gives an equivalent, excellent fit to the measured data, and it is known that a refractive interaction with short ranged repulsion is needed to explain the structure of cross-section data at higher incident energies [4].

Finally, as the data are extremely good, we can apply an error analysis. The cross sections have been measured at many angles over a wide range of momentum transfer and the values have small nonstatistical errors, whence fits with χ^2/F of order unity allow a meaningful statistical error analysis to be applied. Such has been the case with analyses of electron-He atom scattering in the recent past [6] and, in a similar way here, confidence intervals on the potentials obtained by inversion have been found within a WKB approximation (which will yield similar results to a more computationally demanding fully quantal analysis such as that done in Ref. [8]). The interpretation of these intervals is as follows: should another potential exist which fits the cross-section data with the same χ^2/F, then there is about a 60% probability that it will lie within the confidence band shown by the hatched zones in Fig. 4. Clearly there is little overlap between the confidence intervals on the two potentials we have determined by inversion. This displays a nonuniqueness with the chosen method to effect the inversion but, in particular, that associated with the transformation from cross section to scattering function. Of the two potentials, that found starting from initial pole-zero pair values that reflect a conjectured interaction, has given a more physical final result.

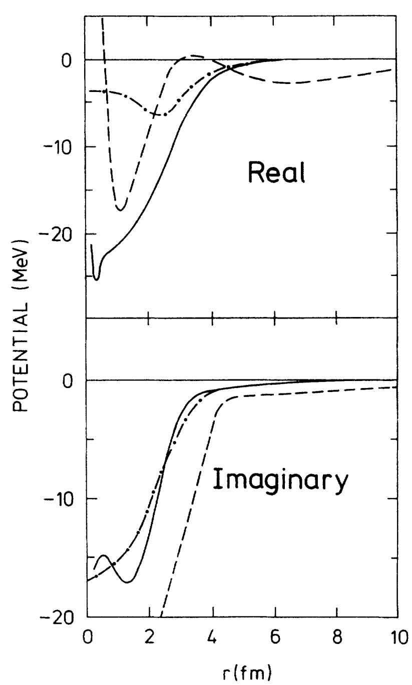

FIG. 3. The real (top) and imaginary (bottom) parts of central potentials for 200 MeV protons on ^{12}C. The dashed and solid curves are the results obtained by inversion and using the set 1 and set 2 parameters in the rational form of the S function, respectively. The dot-dashed curves display a central (DWS) phenomenological interaction.

IV. CONCLUSIONS

A fixed energy quantal inversion method has been used to extract effective local, complex potentials from the elastic scattering differential cross section for 200 MeV protons off of ^{12}C. The associated fits to the measured data are extremely good in each case, and sufficiently so

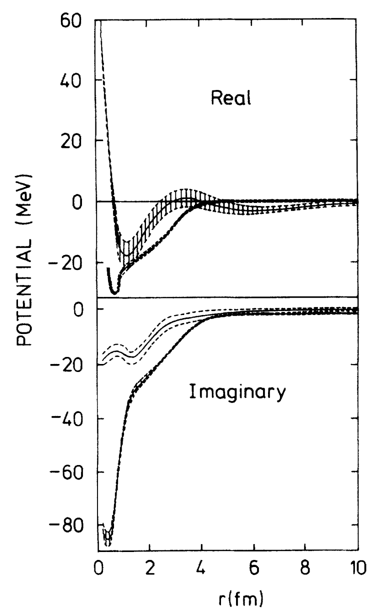

FIG. 4. The real (top) and imaginary (bottom) potentials obtained by inversion of the 200 MeV p-^{12}C cross-section data and the confidence bands on each part. The results found using set 1 parameters are displayed by the hatched curves; those with set 2, by the open lines.

that sensible error analyses of the results could be made.

The procedure used a rational function form for the S function and the complex values of its poles and zeros specified by a χ^2 minimization search to fit the data [3]. Two starting sets of parameter values (of a five pole-zerò pair set) led to two very distinctive and different S functions, both of which gave data fits that were measured by χ^2/F being close to unity and were of similar statistical significance.

The first search started from arbitrary initial values of the parameters in the rational scattering function and led to the final result we have designated as set 1. The second set was obtained from initiating the search with a set of parameter values that reproduce quite well the S function found from solution of the Schrödinger equation with a phenomenological optical model potential [3], which itself gave a reasonable fit to the data. In this second case, the optimal S function had far fewer significant partial wave elements (so far as fitting the cross section is concerned) than for set 1. Quantal inversions of the two rational function forms then were made using a Lipperheide-Fiedeldey theory, and smooth well-behaved complex potentials resulted. That derived from set 1 was not realistic however, being too long ranged and excessively absorptive. The second parameter set (set 2) led to a realistic interaction. It has an imaginary component quite similar to that of the phenomenological potential and a real part that, while more refractive than the phenomenological one, resembles the result found by folding realistic NN g matrices with the density matrices for the ground state of ^{12}C.

Our opinion that the interaction determined from the parameter set 2 is more physical than the one obtained by using the set 1 values, clearly was not based upon the quality of the fit to the cross-section data that the use of each gives. Rather, our choice was based upon a predjudice as to what the true optical model potential should be like, particularly in the range of its action and in the character of its refraction and absorption. The preferred potential is much more like the "best" interactions found by totally phenomenological studies of scattering and also it is much more like the (real) interaction other studies have found by folding "realistic" NN g matrices with nuclear density matrices for ^{12}C.

It would be of help to have (equally well) measured data taken at nearby energies, e.g., at 190–210 MeV, as then one might look for an appropriate energy dependence with a physically realistic candidate inversion potential. One expects some energy dependence with a local potential (that leads to quality fits to elastic scattering data) as that would reflect true nonlocality in the optical potential and due to Pauli effects as well as to the actual nonlocalities existing in the underlying NN g matrices themselves. Possibly there is such quality data at 160 MeV, but that incident energy is just too far from the one of interest (200 MeV) for use to be made of it to delineate between any results one may find by starting with either set 1 or set 2 parameters found herein.

Finally, the quality of the data and the fits to it found by these inverse scattering studies were such that error analyses of the results were feasible. At about 60% confidence, the two inversion potentials had little in common. Clearly then, a bias must be invoked to select physically sensible results from sets of equivalent inversion potentials (in terms of their fit to the data). Notably a bias must be invoked to ensure that the mapping of the cross-section data to S function results in a physically acceptable parametrization.

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