Determination of scattering phase shifts via the generalized unitarity theorem for spin-orbit interactions

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(Received 2 July 1996)

The unitarity conditions upon the scattering amplitudes for the elastic scattering of spin-$\frac{1}{2}$ particles from spin-0 targets at energies below the first inelastic threshold transcribe to a set of coupled nonlinear integral equations for the phase functions of two helicity amplitudes and thence, by simple linkage, to the non-spin-flip and spin-flip scattering amplitudes. From the latter set, by Legendre integrations, one obtains the scattering phase shifts, $\delta_{(l,\, j=l\pm 1/2)}$. Input to the study are the differential cross section and the polarization, $\{(d\sigma/d\Omega)(\theta),P(\theta)\}$. An iterative method of solution based upon Frechét derivatives and with generalized cross validation (GCV) smoothing of the variations between iterates can give convergent, stable, and accurate results. Two test cases, the first built upon a model set of (small) phase-shift values and the second for an optical model calculation of 1-MeV neutrons scattered from an α particle, have been used to demonstrate convergence and accuracy. There are natural ambiguities (fourfold, in fact) for the phase functions of the scattering amplitudes since data are invariant to complex conjugation of, or the Minami transform on, the phase shifts of the mirror data set $\{(d\sigma/d\Omega)(\theta),-P(\theta)\}$, as well as to the combined action of complex conjugation and Minami transformation of the phase shifts given by the initial solution. Those ambiguities are presented herein and are shown not to pose numerical problems in solution, provided the initial guesses are not near to the symmetry ''lines'' of the four solutions, and the GCV process is used to prevent branch flips occurring at scattering angles where the allowed solutions intersect. [S1050-2947(97)03603-2]

PACS number(s): 34.80.−i

I. INTRODUCTION

Phase-shift analyses usually are precursors to the use of inverse scattering methods [1] to obtain (local) interaction potentials from scattering data. With fixed energy inverse scattering problems, knowledge of the phase shifts δ_l at all real positive values of the variable l allows unique determination of the Schrödinger potentials. The first problem then is to specify those phase shifts, first at the physical values and then, by interpolation, for all values of the angular momentum variable. But no technique exists to do that unambiguously. Most commonly, S-matrix fitting procedures are used and usually, therewith, aspects of ill-posedness and of ambiguities due to local minima in the n-parameter hypersurface associated with such procedures are ignored.

Our aim has been to obtain phase shifts by a more global means, namely by using the unitarity (generalized flux) theorem in application to real cases. Below the first nonelastic threshold and for the scattering of spinless particles (or if one simply ignores any spin-dependent attributes in the scattering), this theorem translates to an integral equation to determine the phase function $[\varphi(\theta)]$ of the scattering amplitude $f(\theta)=\sqrt{d\sigma/d\Omega}(\theta)\exp[i\varphi(\theta)]$. A solution to that integral equation not only exists but also, under particular conditions [2], is unique. Furthermore, with one of those conditions (hereafter defined as the Martin condition) being valid, an iterative method of Newton [3] gives that solution. When conditions for uniqueness and stability of solution by an iterated fixed point method are not met, a numerical procedure has been proposed [4,5]. But whatever the chosen method of solution, the cross-section data $(d\sigma/d\Omega)(\theta)$ must be known at all (real) scattering angles. With actual data sets then, interpolation and extrapolation must be used.

For scattering in which spin-orbit interactions are important, the generalized flux theorem leads to coupled integral equations for two unknown phase functions [6], and while there are still conditions for uniqueness of the solution as well as of the stability of fixed-point methods of solution, those conditions are now quite complex in nature. Indeed it would seem that the mathematical complexity of the spin-orbit problem is greater than that of the no-spin-orbit scattering, two-channel system [7], but in practice it is not. In most cases of two-channel scattering, one or more of the required data sets are unavailable. Certainly the problem is more complex than the single-channel equation that we studied recently [4,5] for spinless particle scattering. In fact we ignored spin-orbit effects in the unitarity equations for the systems studied; the process then is an approximation to the coupled equation forms given herein when the polarizations are set to zero at all scattering angles. As with those earlier studies, herein we again ignore specific Coulomb interaction effects by restricting consideration to scattering from systems such that the phase shifts all rapidly decrease with partial wave value. As a realistic case, we consider low-energy neutron–α-particle scattering (n-α), and as with our previous analysis [4] of that scattering, stable solutions cannot be found by using the Newton fixed-point iterative method. So we resort to a method of solution based upon Frechét derivatives. With that approach, we have found the scattering phase functions in both a test case and with input based upon the cross sections and polarizations given by a conventional op-

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tical model calculation for low-energy ($n-\alpha$) scattering [8]. The fourfold ambiguity due to invariance of results based upon both complex conjugation and the Minami transform is studied and the problems such ambiguity may cause in numerical evaluation of the phase shifts are given.

II. UNITARITY AND SPIN-$\frac{1}{2}$–SPIN-0 ELASTIC SCATTERING AMPLITUDES

The scattering amplitudes for a spin-$\frac{1}{2}$ particle elastically scattered from a spin-0 target have the form

$$f_{\tau'\tau}(\mathbf{k}',\mathbf{k})=\chi^{\dagger}_{\tau'}[g(\theta)+\boldsymbol{\sigma}\cdot\mathbf{n}\;\; h(\theta)]\chi_{\tau},\quad \mathbf{n}=\frac{\mathbf{k}\times\mathbf{k}'}{|\mathbf{k}\times\mathbf{k}'|}\;, \tag{1}$$

where χ_τ are Pauli spin functions with spin projections $\tau=\pm1$, and $\mathbf{k}$, $\mathbf{k}'$ are the incoming and outgoing momenta of the projectile ($|\mathbf{k}|=|\mathbf{k}'|=k$). The non-spin-flip and spin-flip amplitudes, $g(\theta)$ and $h(\theta)$, respectively, are defined conventionally by the partial-wave expansions

$$g(\theta)=\frac{1}{2ik}\sum_{l=0}^{\infty}\;[(l+1)S_{l+}+lS_{l-}-(2l+1)]P_l(\cos\theta)\;, \tag{2}$$

$$h(\theta)=\frac{1}{2k}\sum_{l=1}^{\infty}\;[S_{l+}-S_{l-}]P_l^1(\cos\theta)\;.$$

Therein $l\pm$ denote the values $j=l\pm1/2$ and the expansions can be recast in terms of scattering phase shifts since they are given by $\delta_{l\pm}(k)=[1/(2i)]\;\;\ln[S_{l\pm}(k)]$. Likewise, the unitarity condition (the generalized flux theorem) [1], which has the form

$$-2\pi i[f_{\tau'\tau}(\mathbf{k}',\mathbf{k})-f_{\tau\tau'}{}^{*}(\mathbf{k},\mathbf{k}')]$$

$$=k\sum_{\nu}\;\int\; f_{\tau'\nu}(\mathbf{k}',\mathbf{q})f^{*}_{\nu\tau'}(\mathbf{k},\mathbf{q})\;\; d\Omega q\;, \tag{3}$$

may be expressed in terms of the elements $g(\theta)$ and $h(\theta)$, but it is much more convenient to choose spin quantization parallel to $\mathbf{n}$ and transversity amplitudes

$$\widetilde{f}_{\pm,\pm}(\theta)=\left(\frac{1}{k}\right)A_{\pm}(z)\exp(i\Phi_{\pm})=g(\theta)\pm h(\theta),$$

$$\widetilde{f}_{\mp,\pm}(\theta)=0\;. \tag{4}$$

Therein $A_{\pm}(z)$ $[z=\cos(\theta)]$ are dimensionless magnitude functions that can be determined from the unpolarized differential cross section $d\sigma/d\Omega$ and the polarization $P(\theta)$ since

$$k^2A^2_{\pm}(z)=\frac{d\sigma}{d\Omega}(1\pm P)=(|g|^2+|h|^2)\left(1\pm\frac{2\mathrm{Re}(gh^*)}{(|g|^2+|h|^2)}\right)\;. \tag{5}$$

Then if the $A_{\pm}(z)$ can be specified for all scattering angles, the unitarity condition, Eq. (3), constitutes two coupled equations [6] for the phase functions $\Phi_{\pm}(\theta)$. Those equations are nonlinear and can be specified in a convenient form, by assuming $\Phi_+,\Phi_-\in C[-1,1]$, defining $\Phi\equiv\binom{\Phi_+}{\Phi_-}$, and then considering an operator $F\equiv\binom{F_+}{F_-}$ whose components F_+, F_- are

$$F_+[\Phi]\equiv A_+(z)\sin[\Phi_+(z)]+A_-(z)\sin[\Phi_-(z)]-K_1(z)\;, \tag{6}$$

and

$$F_-[\Phi]\equiv A_+(z)\cos[\Phi_+(z)]-A_-(z)\cos[\Phi_-(z)]-K_2(z)\;, \tag{7}$$

where, with $\Theta(K)$ being the Heaviside function,

$$K_1(z)=\int\int\frac{dx\;\;dy\;\;\Theta(K)}{4\pi\sqrt{K}}\sum_{\tau,\tau'=\pm1}A_\tau(x)A_{\tau'}(y)\left(1-\tau\tau'\frac{xy-z}{\overline{x}\;\overline{y}}\right)\cos[\Phi_\tau(x)-\Phi_{\tau'}(y)] \tag{8}$$

and

$$K_2(z)=\int\int\frac{dx\;\;dy\;\;\Theta(K)}{4\pi\sqrt{K}}\sum_{\tau,\tau'=\pm1}A_\tau(x)A_{\tau'}(y)\left\{\left(\tau\tau'\frac{K}{\overline{x}\;\overline{y}\;\overline{z}}\right)\cos[\Phi_\tau(x)-\Phi_{\tau'}(y)]\right.$$
$$\left.+\left(\tau\frac{xz-y}{\overline{x}\;\overline{z}}-\tau'\frac{yz-x}{\overline{y}\;\overline{z}}\right)\sin[\Phi_\tau(x)-\Phi_{\tau'}(y)]\right\}\;, \tag{9}$$

with

$$K=1-x^2-y^2-z^2+2xyz$$

and

$$\overline{a}=\sqrt{1-a^2}\quad\text{for}\quad a\in\{-1<x,y,z<1\}\;.$$

The unitarity equations [6] then have the form

$$F[\Phi]=\begin{pmatrix}0\\0\end{pmatrix}, \tag{10}$$

which is useful in seeking a solution by a modification to the fixed-point iterative method of Newton [1]. That modified method [4,5] involves the Frechét derivative of F, which is given by

$$F'_{\Phi}[h]=\begin{pmatrix} \dfrac{\partial F_+}{\partial\Phi_+}[h_+]+\dfrac{\partial F_+}{\partial\Phi_-}[h_-] \\ \dfrac{\partial F_-}{\partial\Phi_+}[h_+]+\dfrac{\partial F_-}{\partial\Phi_-}[h_-] \end{pmatrix}, \quad h\equiv\begin{pmatrix}h_+\\h_-\end{pmatrix} \quad , \tag{11}$$

where, with $h_\pm$ being the functionals of variation,

$$\begin{aligned}\frac{\partial F_+}{\partial\Phi_+}[h_+]=&\,h_+(z)A_+(z)\cos[\Phi_+(z)]-\int\int\frac{dx\ \ dy\ \ \Theta(K)}{4\pi\sqrt{K}}\\ &\times\left\{-A_+(x)A_+(y)\left(1-\frac{xy-z}{\bar{x}\ \bar{y}}\right)\ \sin[\Phi_+(x)-\Phi_+(y)]\ \ [h_+(x)-h_+(y)]-A_+(x)A_-(y)\left(1+\frac{xy-z}{\bar{x}\ \bar{y}}\right)\right.\\ &\left.\times\sin[\Phi_+(x)-\Phi_-(y)]\ \ h_+(x)-A_-(x)A_+(y)\left(1+\frac{xy-z}{\bar{x}\ \bar{y}}\right)\ \sin[\Phi_+(y)-\Phi_-(x)]\ \ h_+(y)\right\}\\ =&\,h_+(z)A_+(z)\cos[\Phi_+(z)]+2\int\int\frac{dx\ \ dy\ \ \Theta(K)}{4\pi\sqrt{K}}A_+(x)h_+(x)\left\{A_+(y)\left(1-\frac{xy-z}{\bar{x}\ \bar{y}}\right)\sin[\Phi_+(x)-\Phi_+(y)]\right.\\ &\left.+A_-(y)\left(1+\frac{xy-z}{\bar{x}\ \bar{y}}\right)\sin[\Phi_+(x)-\Phi_-(y)]\right\}\quad ,\end{aligned} \tag{12}$$

$$\begin{aligned}\frac{\partial F_+}{\partial\Phi_-}[h_-]=&\,h_-(z)A_-(z)\cos[\Phi_-(z)]+2\int\int\frac{dx\ \ dy\ \ \Theta(K)}{4\pi\sqrt{K}}A_-(x)h_-(x)\left\{A_-(y)\left(1-\frac{xy-z}{\bar{x}\ \bar{y}}\right)\sin[\Phi_-(x)-\Phi_-(y)]\right.\\ &\left.+A_+(y)\left(1+\frac{xy-z}{\bar{x}\ \bar{y}}\right)\sin[\Phi_-(x)-\Phi_+(y)]\right\}\quad ,\end{aligned} \tag{13}$$

$$\begin{aligned}\frac{\partial F_-}{\partial\Phi_+}[h_+]=&-h_+(z)A_+(z)\sin[\Phi_+(z)]-\int\int\frac{dx\ \ dy\ \ \Theta(K)}{4\pi\sqrt{K}}\left[A_+(x)A_+(y)\left\{-\frac{K}{\bar{x}\ \bar{y}\ \bar{z}}\sin[\Phi_+(x)-\Phi_+(y)]\right.\right.\\ &\left.\times[h_+(x)-h_+(y)]+\left(\frac{xz-y}{\bar{x}\ \bar{z}}-\frac{yz-x}{\bar{y}\ \bar{z}}\right)\cos[\Phi_+(x)-\Phi_+(y)][h_+(x)-h_+(y)]\right\}\\ &+A_+(x)A_-(y)\left\{\frac{K}{\bar{x}\ \bar{y}\ \bar{z}}\sin[\Phi_+(x)-\Phi_-(y)]\ \ h_+(x)+\left(\frac{xz-y}{\bar{x}\ \bar{z}}+\frac{yz-x}{\bar{y}\ \bar{z}}\right)\ \cos[\Phi_+(x)-\Phi_-(y)]\ \ h_+(x)\right\}\\ &\left.+A_-(x)A_+(y)\left\{\frac{K}{\bar{x}\ \bar{y}\ \bar{z}}\sin[\Phi_+(y)-\Phi_-(x)]\ \ h_+(y)+\left(\frac{xz-y}{\bar{x}\ \bar{z}}+\frac{yz-x}{\bar{y}\ \bar{z}}\right)\cos[\Phi_+(y)-\Phi_-(x)]\ \ h_+(y)\right\}\right]\\ =&-h_+(z)A_+(z)\sin[\Phi_+(z)]-2\int\int\frac{dx\ \ dy\ \ \Theta(K)}{4\pi\sqrt{K}}A_+(x)h_+(x)\left[A_+(y)\left\{-\frac{K}{\bar{x}\ \bar{y}\ \bar{z}}\sin[\Phi_+(x)-\Phi_+(y)]\right.\right.\\ &\left.+\left(\frac{xz-y}{\bar{x}\ \bar{z}}-\frac{yz-x}{\bar{y}\ \bar{z}}\right)\cos[\Phi_+(x)-\Phi_+(y)]\right\}+A_-(y)\left\{\frac{K}{\bar{x}\ \bar{y}\ \bar{z}}\sin[\Phi_+(x)-\Phi_-(y)]\right.\\ &\left.\left.+\left(\frac{xz-y}{\bar{x}\ \bar{z}}+\frac{yz-x}{\bar{y}\ \bar{z}}\right)\cos[\Phi_+(x)-\Phi_-(y)]\right\}\right]\quad ,\end{aligned} \tag{14}$$

and

$$\frac{\partial F_-}{\partial \Phi_-}[h_-]=h_-(z)A_-(z)\sin[\Phi_-(z)]-2\int\int\frac{dx\ \ dy\ \ \Theta(K)}{4\pi\sqrt{K}}A_-(x)h_-(x)\Bigg[A_-(y)\Bigg\{-\frac{K}{\overline{x}\,\overline{y}\,\overline{z}}\sin[\Phi_-(x)-\Phi_-(y)]$$
$$-\left(\frac{xz-y}{\overline{x}\,\overline{z}}-\frac{yz-x}{\overline{y}\,\overline{z}}\right)\cos[\Phi_-(x)-\Phi_-(y)]\Bigg\}+A_+(y)$$
$$\times\Bigg\{\frac{K}{\overline{x}\,\overline{y}\,\overline{z}}\sin[\Phi_-(x)-\Phi_+(y)]-\left(\frac{xz-y}{\overline{x}\,\overline{z}}+\frac{yz-x}{\overline{y}\,\overline{z}}\right)\cos[\Phi_-(x)-\Phi_+(y)]\Bigg\}\Bigg]\ . \tag{15}$$

The modified Newton method of solution necessitates that one solves the system of two coupled linear functional equations for two components of Φ^{n+1}, viz.,

$$F[\Phi^n]+F'_{\Phi^n}[\Phi^{n+1}-\Phi^n]=0. \tag{16}$$

If the integrals (over y) are approximated by means of a quadrature formula, these equations reduce to a linear system with matrix form:

$$\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22}\end{pmatrix}\begin{pmatrix} h_+ \\ h_-\end{pmatrix}=F. \tag{17}$$

In the process of solution it is useful to incorporate a set of useful limits of the coupled equations that result from the constraints specified by Alvarez-Estrada and Carreras [6], i.e., as $z\ \to\pm 1$, $\Theta(K)/\sqrt{K}\to\pi\delta(x\mp y)$. Those limits are as follows:

(1) At $z=1$, Eq. (6) leads to the optical theorem

$$\sin[\Phi_\pm(1)]=\frac{1}{4A_+(1)}\int_{-1}^{1}[A_+^2(x)+A_-^2(x)]\ \ dx\ \ . \tag{18}$$

(2) At $z=-1$, one has

$$\frac{\partial F_+}{\partial \Phi_+}[h_+]=h_+(-1)A_+(-1)\cos[\Phi_+(-1)]$$
$$+\int_{-1}^{1}A_+(x)h_+(x)A_-(-x)$$
$$\times\sin[\Phi_+(x)-\Phi_-(-x)]\ \ dx\ \ , \tag{19}$$

$$\frac{\partial F_+}{\partial \Phi_-}[h_-]=h_-(-1)A_-(-1)\cos[\Phi_-(-1)]$$
$$+\int_{-1}^{1}A_-(x)h_-(x)A_+(-x)$$
$$\times\sin[\Phi_-(x)-\Phi_+(-x)]\ \ dx\ \ , \tag{20}$$

$$\frac{\partial F_-}{\partial \Phi_+}[h_+]=-h_+(-1)A_+(-1)\sin[\Phi_+(-1)]\ \ ,$$

and

$$\frac{\partial F_-}{\partial \Phi_-}[h_-]=h_-(-1)A_-(-1)\sin[\Phi_-(-1)]\ \ . \tag{21}$$

(3) At $x=-1$ one has

$$M_{11}(i,1)\ =A_+(z_i)\cos[\Phi_+(z_i)]\delta_{i1}+\frac{A_+(-1)}{2}$$
$$\times\{A_+(-z_i)\sin[\Phi_+(-1)-\Phi_+(-z_i)]$$
$$+A_-(-z_i)\sin[\Phi_+(-1)-\Phi_-(-z_i)]\}\ \ ,$$

$$M_{12}(i,1)\ =A_-(z_i)\cos[\Phi_-(z_i)]\delta_{i1}+\frac{A_-(-1)}{2}$$
$$\times\{A_-(-z_i)\sin[\Phi_-(-1)-\Phi_-(-z_i)]$$
$$+A_+(-z_i)\sin[\Phi_-(-1)-\Phi_+(-z_i)]\}\ \ ,$$

$$M_{21}(i,1)\ =-A_+(z_i)\sin[\Phi_+(z_i)]\ \ \delta_{i1}\ \ ,$$

and

$$M_{22}(i,1)\ =A_-(z_i)\sin[\Phi_-(z_i)]\ \ \delta_{i1}\ \ . \tag{22}$$

Once the phase functions of the transversity amplitudes have been fixed, so also are the scattering amplitudes, $g(\theta)$ and $h(\theta)$, from which the scattering functions (equivalently the phase shifts) can be determined by the Legendre integrations

$$S_{l+}-1=ik\int_{-1}^{1}g(x)P_l(x)dx$$
$$+\ \ \frac{k}{l+1}\int_{-1}^{1}h(x)P_l^1(x)dx, \tag{23}$$

$$S_{l-}-1=ik\int_{-1}^{1}g(x)P_l(x)dx-\frac{k}{l}\int_{-1}^{1}h(x)P_l^1(x)dx$$

for $l\neq 0$. For the s-wave case, only the equation for S_{0+} has relevance.

III. NATURAL AMBIGUITIES OF THE PHASE FUNCTIONS

Alvarez-Estrada *et al.* [6,7] have specified the set of uniqueness conditions for a solution, $\Phi\equiv\{\Phi_+(\theta),\Phi_-(\theta)\}$

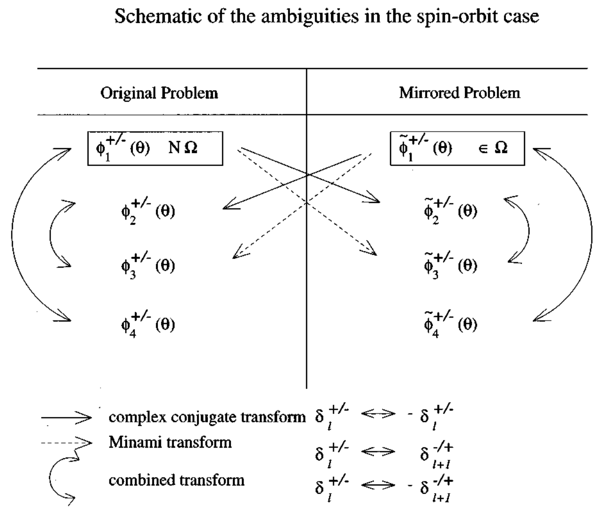

FIG. 1. A schematic diagram of the natural ambiguities with the phase functions of the (transversity) scattering amplitudes from spin-$\frac{1}{2}$ particles scattering off spin-0 targets. One solution of each of the given and mirrored problem has been assumed to lie in the function space Ω.

of the unitarity equations for the problem specified by the data set $\{(d\sigma/d\Omega)(\theta),P(\theta)\}$. Those conditions are quite complex and identify the solution to be unique within a function domain Ω. Such a solution, if it exists, we designate as $\Phi^{(1)}$. There is also then a solution to the "mirrored" problem specified by the data set $((d\sigma/d\Omega)(\theta),-P(\theta))$, which we designate hereafter by $\widetilde{\Phi}^{(1)}$.

Natural ambiguities to those solutions exist, identified by application of the complex conjugate, the Minami, and the combination of the complex conjugate and Minami transformations. The complex conjugation transform equates to changing the signs of all of the phase shifts $\delta_{l\pm}$ one obtains from the phase functions $\widetilde{\Phi}^{(1)}$ (and from $\Phi^{(1)}$ for the mirrored problem), which are given by

$$\Phi^{(2)}=\begin{pmatrix}\Phi_+^{(2)}\\ \Phi_-^{(2)}\end{pmatrix}=\begin{pmatrix}\pi-\widetilde{\Phi}_-^{(1)}\\ \pi-\widetilde{\Phi}_+^{(1)}\end{pmatrix}\quad, \tag{24}$$

and similarly for $\widetilde{\Phi}^{(2)}$. The Minami transform is effected by an interchange of phase shift sets by $\delta_{l\pm}\Leftrightarrow\delta_{(l+1)\mp}$ or by specification of the new phase functions, $\Phi^{(3)}$, by

$$\Phi^{(3)}=\begin{pmatrix}\Phi_+^{(3)}\\ \Phi_-^{(3)}\end{pmatrix}=\begin{pmatrix}\widetilde{\Phi}_-^{(1)}-\theta\\ \widetilde{\Phi}_+^{(1)}+\theta\end{pmatrix}, \tag{25}$$

and similarly for $\widetilde{\Phi}^{(3)}$. A fourth possible solution results from the combination of transforms whence we find the phase functions $\Phi^{(4)}$ (and similarly $\widetilde{\Phi}^{(4)}$) from

$$\Phi^{(4)}=\begin{pmatrix}\Phi_+^{(4)}\\ \Phi_-^{(4)}\end{pmatrix}=\begin{pmatrix}\pi-\Phi_+^{(1)}-\theta\\ \pi-\Phi_-^{(1)}+\theta\end{pmatrix}\quad. \tag{26}$$

These natural ambiguities and the links between them are shown schematically in Fig. 1 wherein a finding of Alvarez-Estrada *et al.* is stressed; namely, if $\Phi_\pm^{(1)}\in\Omega$, so also is $\widetilde{\Phi}_\pm^{(1)}$ but none of the other solutions are. We show herein that the combination of complex conjugation and Minami transformation gives a new phase function set $\Phi_\pm^{(4)}$ and $\widetilde{\Phi}_\pm^{(4)}$ for the original and the mirrored data sets, respectively, while the two other possible solutions to the original problem require the complex conjugation or the Minami transformation of the solution to the mirrored problem, and vice versa.

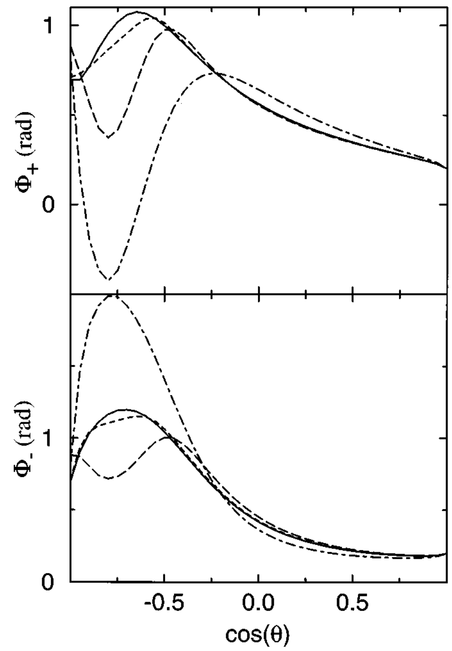

FIG. 2. The iteration results of the modified Newton method applied to the simulated data of spin-0–spin-$\frac{1}{2}$ scattering. Various iterate results for the phase functions Φ_+ and Φ_- are shown in the top and bottom panels, respectively. The first, second, third, and final (fourth) iterates are displayed by the dot-dashed, long-dashed, short-dashed, and solid curves, respectively.

IV. RESULTS OF TEST CALCULATIONS

A. Simulated data case

The method has been tested with simulated data that were generated from the phase shifts $\delta_0=20°$, $\delta_{1+}=10°$, $\delta_{1-}=9°$, $\delta_{2+}=3°$ and $\delta_{2-}=2°$. For this test case, the method converges. We display in Fig. 2 the results [for $\Phi_\pm^{(1)}(\theta)$] found by using the Frechét derivative and with the initial functions being constants. After four iterations the phase functions Φ_+ and Φ_- converged with the accuracy of 0.2% error. In Fig. 2 the first, second, third, and final (fourth) iterates are shown by the dot-dashed, long-dashed, short-dashed, and solid curves, respectively. Note that the process we use includes smoothing by generalized cross validation (GCV) [9] between each iterate. That smoothing was found necessary to ensure convergence of the solution for the phase function from the generalized flux theorem for the scattering of spinless particles [5] and it remains so with these studies. Notably, the smoothing ensures that branch flips in solutions do not occur, i.e., that for the scattering angles in the vicinity of the crossing of the desired phase function with an alternative solution, the numerics maintain convergence to the desired one and not to the alternative. The final iterate coincides so very well with the exact solution that the latter is not displayed separately.

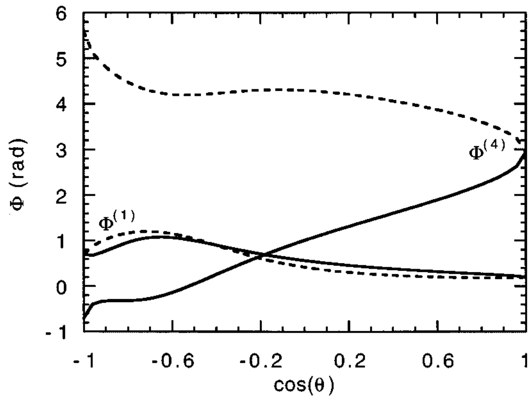

FIG. 3. The $\Phi_{\pm}^{(1)}$ and $\Phi_{\pm}^{(4)}$ solutions of the nonlinear equations based upon the simulated data set for spin-0–spin-$\frac{1}{2}$ scattering. The $+$ and $-$ solutions are displayed by the solid and dashed curves, respectively.

The coupled equations were solved also by using as the initial guess for the phase functions the complex conjugate and Minami transform of the initial conditions (as used above). The results of the iterated solution, $\Phi_{\pm}^{(4)}(\theta)$, are given in Fig. 3 and they are compared with the $\Phi_{\pm}^{(1)}(\theta)$ solutions. There is a branch point for the Φ_{+} solutions as the two functions $\Phi_{+}^{(1)}$ and $\Phi_{+}^{(4)}$ cross near 100° scattering angle. No such branch point exists for the Φ_{-} solutions, however. In this case, the branch point caused no difficulties with the numerical solutions of the type encountered in earlier analyses [5] in part due to GCV smoothing between iterations. But the initial guess, Φ^{0}, must not be taken at or near to the symmetry lines,

$$\Phi^{0}=\begin{pmatrix}\Phi_{+}^{0}\\ \Phi_{-}^{0}\end{pmatrix}\neq\begin{pmatrix}\dfrac{\pi}{2}-\dfrac{1}{2}\theta\\ \dfrac{\pi}{2}+\dfrac{1}{2}\theta\end{pmatrix}\quad, \tag{27}$$

as then the problem becomes singular, with the probabilities of the solutions converging to $\Phi^{(1)}$ and $\Phi^{(4)}$ nearly equivalent at all scattering angles.

B. The case of 1 MeV n-α scattering

1. The direct data set {(dσ/dΩ)(θ),P(θ)}

We have chosen this case because in an earlier study [5] in which spin-orbit coupling effects were ignored, the unitarity equations could be solved without numerical ambiguity. For convenience, to specify the data at all scattering angles, we have used the phase shifts for 1 MeV n-α scattering as given by the optical model analysis that was made by Satchler *et al.* [8]. Not only does this give a good fit to the actual measured data but also provides us with the ''exact'' phase functions against which we can compare the results of our unitarity based analysis.

Our first (of two) guess for the initial phase functions was to assume the linear form [in $z=\cos(\theta)$]

$$\Phi_{\pm}^{0}=\varphi_{\pm}^{(0)}+\left(\frac{\varphi_{\pm}^{(m)}-\varphi_{\pm}^{(0)}}{2}\right)(1+z)\quad. \tag{28}$$

TABLE I. The 1-MeV n-α scattering phase shifts as calculated from the Satchler *et al.* [8] optical potential (designated ''orig'') and as recalculated (''rec'') from the phase functions $\Phi_{\pm}^{(1)}$, found by using the linear initial guess functions of Eq. (28).

l	$\delta_l^{+,\mathrm{orig}}$	$\delta_l^{-,\mathrm{orig}}$	$\delta_l^{+,\mathrm{rec}}$	$\delta_l^{-,\mathrm{rec}}$
0	2.707		2.70683	
1	1.007	0.091	1.00688	0.09093
2	0.001	0.0001	0.000104	−0.00005
3	0.000	0.000	−0.00009	0.00008

With the parameters taken as

$$\varphi_{+}^{(0)}=4.28\,,$$

$$\varphi_{-}^{(0)}=1.21\,,$$

$$\varphi_{+}^{(m)}=-2.0\,, \tag{29}$$

$$\varphi_{-}^{(m)}=1.21\,,$$

the solutions are identified as $\Phi^{(1)}$. From those phase functions, by Legendre integration of the associated complex scattering amplitude, we obtained the ''recalculated'' phase shifts that are compared in Table I with the ''original'' ones, i.e., obtained from the optical potential of Satchler *et al.* [8]. The agreement is very good, being of the order of 1 part per 1000 for the important partial waves. The initial phase functions and the final results are displayed in Fig. 4 by the dashed and the solid curves, respectively. The changes wrought by the iterative method of solution are significant as seen by the variation in cross section and polarization for this scattering given in Fig. 5. Therein the cross section and polarization shown by the dashed curves are the result of using the phase shifts extracted from the initial phase function guess and used in the partial wave summations of Eqs. (2) while those displayed by the solid curves are the results

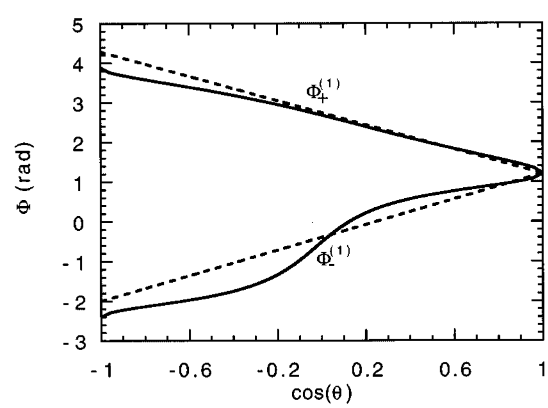

FIG. 4. The initial and final, $\Phi^{(1)}$, phase functions for 1-MeV n-α scattering and based upon the optical potential ''data'' of Satchler *et al.* [8]. The initial guess functions given by Eq. (28) are displayed by the dashed curves while the solid curves portray the results of our calculations. The latter coincide extremely well with the ''exact'' values of the Satchler optical potential.

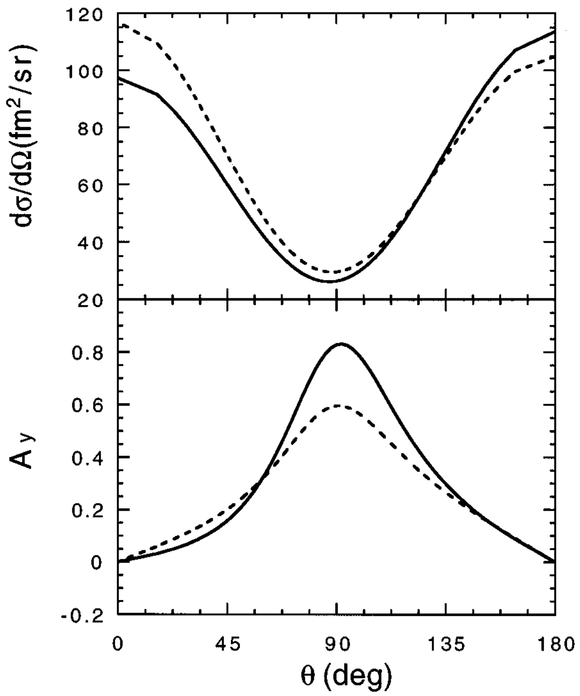

FIG. 5. The differential cross sections (top) and polarizations (bottom) for 1-MeV n-α scattering as calculated from the phase shifts specified by using the initial guess phase function of Eq. (28) and from the phase shifts found using the phase function solution of the generalized flux equation. The former are shown by the dashed curves while the latter, depicted by the solid curves, are in very good agreement with the calculated results of Satchler *et al.* [8].

found using the final (40th) iterate. The latter coincide very precisely with the calculated results of Satchler *et al.* [8], the input to our calculations.

The second starting phase guess functions were those given by the complex conjugation and Minami transformation of those in Eq. (28), viz.,

$$\Phi_{\pm}^{0\prime}=\pi-\Phi_{\pm}^{0}\mp\tfrac{1}{2}\theta \quad . \tag{30}$$

With the same parameter set, Eq. (29), we sought solution of the phase functions $\Phi_{\pm}^{(4)}$. The phase shifts then extracted by Legendre integration of the resultant scattering amplitudes are compared with the complex conjugated, Minami transformed set of Satchler *et al.* [8] in Table II. Again the recalculated results agree with the ''data'' to a few parts per thousand for the important partial waves. The final phase functions are compared with the initial ones for this case and with the original, $\Phi_{\pm}^{(1)}$, quantities, in Fig. 6. Therein the + and − phase functions are shown in the top and bottom segments, respectively. The initial guess variations are shown by the dashed lines while the results of our calculations are shown by the solid curves. The symmetry lines between the two solution sets are shown by the small dashed curves. Those symmetry lines also pertain to the two other possible solutions of the coupled nonlinear equations for the phase functions, and which are discussed in the next section. In this case, the solutions $\Phi_{+}^{(1)}$ and $\Phi_{+}^{(4)}$ intersect near 25° for the scattering angle at which point numerical problems with ambiguity of solution could result. With GCV smoothing between iterations, the process converged to the ''exact'' results. There is no such concern with the Φ_{-} phase solutions though as the trial guesses and final results for $\Phi_{-}^{(1)}$ and $\Phi_{-}^{(4)}$ do not cross.

TABLE II. The 1-MeV n-α scattering phase shifts as calculated from the Satchler *et al.* [8] optical potential and after using the complex conjugation and Minami transformations (designated ''orig'') and those recalculated (''rec'') from the phase functions $\Phi_{\pm}^{(4)}$, found by using the transforms of the linear initial guess functions of Eq. (28).

l	$\delta_l^{+,\mathrm{orig}}$	$\delta_l^{-,\mathrm{orig}}$	$\delta_l^{+,\mathrm{rec}}$	$\delta_l^{-,\mathrm{rec}}$
0	−0.091		−0.0911	
1	−0.0001	−2.707	−0.0004	−2.7070
2	0.000	−1.000	0.0002	−1.0058
3	0.000	−0.001	−0.0003	−0.0009

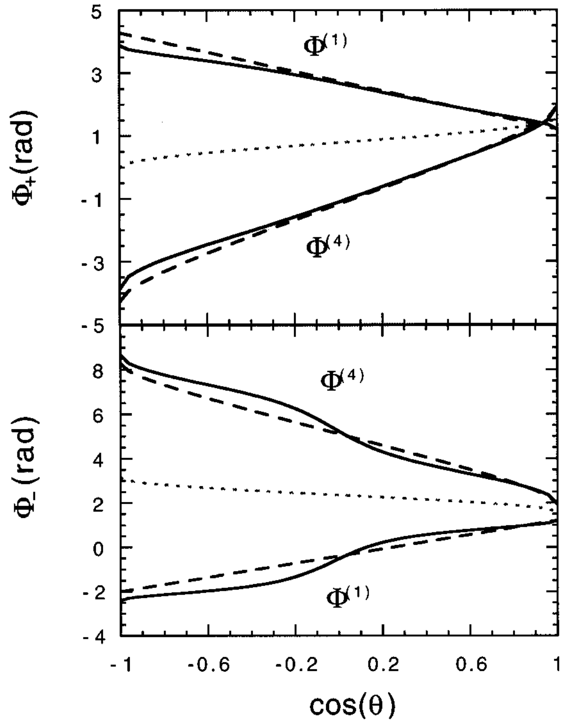

FIG. 6. The (+) (top) and (−) (bottom) phase solutions of $\Phi^{(1)}$ and $\Phi^{(4)}$ as labeled. The starting (guess) phase functions are portrayed by the dashed lines while the final solutions are shown by the solid curves. Those final solutions are in excellent agreement with the ''exact'' ones (original and complex conjugate plus Minami transformed) specified by the Satchler *et al.* [8] scattering phase shifts. The symmetry lines of these solutions are displayed by the small dashed lines in these figures.

2. The mirror data set $\{(d\sigma/d\Omega)(\theta),-P(\theta)\}$

Two more phase functions for the scattering amplitudes of the $\{(d\sigma/d\Omega)(\theta),P(\theta)\}$ data set are associated with the phase functions $\Phi^{(2)}$ and $\Phi^{(3)}$, and are given by the complex conjugate and the Minami transform of the solution with the mirror problem data set $\{(d\sigma/d\Omega)(\theta),-P(\theta)\}$, i.e., $\tilde{\Phi}^{(1)}$, respectively. The mirror problem was solved using the same

TABLE III. The first few partial wave phase shifts obtained from the four phase function solutions associated with the actual $\{(d\sigma/d\Omega)(\theta),P(\theta)\}$ and mirrored $\{(d\sigma/d\Omega)(\theta),-P(\theta)\}$ data sets.

Solution	l	δ_l^+(orig)	δ_l^-(orig)	Solution	l	δ_l^+(mirror)	δ_l^-(mirror)
$\Phi_\pm^{(1)}$	0	2.7070		$\Phi_\pm^{(1)}$	0	0.1000	
	1	1.0070	0.9100		1	1.0420	0.0019
	2	0.0010	0.0001		2	−0.1820	0.0102
	3	0.0000	0.0000		3	0.0440	−1.0560
$\Phi_\pm^{(2)}$	0	−0.1000		$\tilde{\Phi}_\pm^{(2)}$	0	−2.7070	
	1	−1.0420	−0.0019		1	−1.0070	−0.9100
	2	0.1820	−0.0102		2	−0.0010	−0.0001
	3	−0.0440	1.0560		3	0.0000	0.0000
$\Phi_\pm^{(3)}$	0	0.0019		$\tilde{\Phi}_\pm^{(3)}$	0	0.9100	
	1	0.0102	0.1000		1	0.0001	2.7070
	2	−1.560	1.042		2	0.0000	1.0070
	3	0.0000	−0.1820		3	0.0000	0.0010
	4	0.0000	0.0440		4	0.0000	0.0000
$\Phi_\pm^{(4)}$	0	−0.9100		$\tilde{\Phi}_\pm^{(4)}$	0	−0.0019	
	1	−0.0001	−2.7070		1	−0.0102	−0.1000
	2	0.0000	−1.0070		2	1.0560	−1.0420
	3	0.0000	−0.0010		3	0.0000	0.1820
	4	0.0000	0.0000		4	0.0000	−0.0440

linear initial conditions. The result is quite different from the phase function found when either the complex conjugation or the Minami transform is made upon the Satchler phase shifts. In those cases the phase functions we identify as $\tilde{\Phi}^{(2)}$ and $\tilde{\Phi}^{(3)}$, respectively. Then by using these phase functions for the ''data'' set, the phase shifts that result are compared with those extracted from the $\Phi^{(1)}$ and $\Phi^{(4)}$ functions in Table III. When used in the appropriate partial wave summations, Eq. (2), all four sets give equivalent fits to the cross section and polarization of the optical potential calculation.

C. The case of vanishing polarization

In the case of vanishing (or ignored) polarization, the four solutions for the phase function remain, but two are degenerate. Those two phase functions are distinct, however, and when used to specify the complete scattering amplitudes in the Legendre integrations, lead to distinctly different sets of phase shift values. The phase shifts, $\delta_{l\pm}$, are distinct but still give zero polarization when used in the partial wave summations for the scattering amplitudes, Eqs. (2). Thus treating spin-$\frac{1}{2}$–spin-0 scattering, ignoring polarization and equating to the problem of spinless particle scattering [5], overlooks a natural ambiguity of the phase function.

V. CONCLUSIONS

The requirements that scattering functions for quantal scattering at energies below the first inelastic threshold be unitary have been used to specify a process to extract complex scattering amplitudes from the data set of the differential cross section and polarization. The generalized unitarity equations for the scattering of spin-$\frac{1}{2}$ particles from spin-0 targets give a coupled set of equations for the phase functions of two helicity amplitudes from which those of the spin-flip and non-spin-flip scattering amplitudes can be specified. Then, scattering phase shifts $\delta_{l\pm}$ can be deduced by Legendre integrations. This method is more rigorous than conventional phase-shift analyses of the same data but there are known ambiguities of the solution. Four natural phase functions are possible with such scattering as data are invariant under complex conjugation and the Minami transformation. The other two allowed solutions result from applying the complex conjugation and the Minami transformation separately upon solutions of the mirror problem. For vanishing polarization, the fourfold ambiguity still exists but the solutions are pairwise degenerate.

We have performed test calculations of the spin-orbit scattering problem. First we used trial partial wave phase shifts. The ambiguous phase function solutions were investigated and found not to cause numerical instabilities as they did not intersect with the original ones at any scattering angle. Hence no branch point ambiguity existed in this first test problem to cause difficulties with numerics. The phase functions of the second test case did in fact overlap. We chose as the ''exact'' results against which to assess our method of solution the phase functions specified by the scattering phase shifts as given by a conventional optical model potential calculation for 1-MeV neutrons scattered from the α particle.

With initial guesses not too different from the exact results, and certainly by avoiding the symmetry ''line'' of the possible (four) solutions as the initial guess, the method gave stable convergent solutions. It is important to note that generalized cross validation was used to smooth variation between iterates in the method of solution (of the coupled, nonlinear integral equations for the phases of the helicity amplitudes), from which the proper spin-flip and non-spin-flip amplitudes for the scattering were obtained and the ''exact'' phase shifts reproduced by appropriate Legendre integration. The mirror problem was also solved and the three other natural ambiguity solutions for the phase functions specified. The numerical procedure was found to be stable and to converge upon the chosen form of solution even when those phase functions intersected with one or more of the alternatives.

With an interpolation or extrapolation scheme to specify the differential cross section and polarization for spin-$\frac{1}{2}$–spin-0 particle scattering at all scattering angles, we have a method to specify the scattering phase shifts, $\delta_{l\pm}$ at energies to threshold. Thereafter, analyticity with a model prescription for flux loss, or by solution of the additional coupled channel problem, we may seek the most physical phase shift values for the scattering at higher energies.

ACKNOWLEDGMENTS

This research was supported by grants from the Australian Research Committee, from the Austrian Mobilitätsstipendium für Doktoratsabsolventen der Akademisch-Sozialen Arbeitsgemeinschaft Österreichs, and from the Fonds zur Förderung der wissenschaftlichen Forschung in Österreich, Project No. P10467–PHY. H.H. gratefully acknowledges the support of the Akademisch-Sozialen Arbeitsgemeinschaft Österreichs by which his research visit to Melbourne was made possible and the hospitality of the School of Physics during his time there. We thank Dr. H. Leeb for his helpful critical review of our manuscript prior to its submission for publication.

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