Improved spin-orbit inversion method

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We report modifications to an inversion procedure by which central and spin-orbit potentials can be determined starting with scattering phase shifts given at a fixed energy. The formalism can be used to analyze data from the scattering of projectiles with arbitrary spin and the procedure we adopt gives more accurate results than obtained before with this method. [S1050-2947(98)02412-3]

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The spin-orbit interaction is an important feature of many scattering systems ranging from electron-atom to nuclear heavy-ion collisions. When spin-$\frac{1}{2}$ particles are scattered from unpolarized targets, the usual measured data are the differential cross sections and Sherman functions or the analyzing powers. Those data define the helicity amplitudes for scattering from which one can extract sets of scattering phase shifts that depend on the orbital and total angular momentum quantum numbers (ℓ, j). Thereby most methods of fixed energy, quantal inversion [1] that have been used to date to analyze actual scattering data [2] are not appropriate as they are based upon an equation of motion in which the scattering potentials are not dependent upon ℓ, i.e., such as the spin-orbit interaction. We note that there exist numerical inversion techniques, such as the totally phenomenological (optical model potential) approach to the iterative-perturbative methods of Mackintosh and Cooper [3], to ascertain spin-orbit interactions. However, our interest lies with global inverse scattering theories and for those interpolation formulas [4] provide the connection that, in principle, allows inversion of phase shift sets to extract both central and spin-orbit potentials. Hooshyar [5] has used the Sabatier interpolation formulas to construct such an inversion method and Huber and Leeb [6] have investigated an approach to this problem in some detail. Likewise, an approximate scheme [7] has been used with some success [8] to analyze neutron-α particle scattering data in particular. However, a most promising method has been developed [9]. It is also based upon the Sabatier interpolation formulas, but reduces the process of inversion to finding the solution of a system of linear-algebraic equations.

In this Brief Report we develop the linear-algebraic approach [9] to give a formalism suitable for the analysis of quantal scattering of spin-$\frac{1}{2}$ particles, such as of electrons from atoms and nucleons from nuclei. We demonstrate that suitability by reanalyzing the nuclear scattering problem studied with the original scheme [9] and ones extended to include Coulomb as well as flux loss effects. The results we find are in better agreement with the test potentials than were those obtained previously [9], as well as being for potentials of the form used in standard phenomenological analyses of actual scattering data.

In this study we assume that the scattering of a spin-S particle with center-of-mass energy E can be specified from solutions of partial-wave Schrödinger equations that have the form

$$\left[\frac{\partial^2}{\partial r^2}+\frac{2\mu E}{\hbar^2}-\frac{\ell(\ell+1)}{r^2}-\frac{2\mu}{\hbar^2}\{V_c(r)+V_{\rm so}(r)\langle 2\mathbf{L}\cdot\mathbf{S}\rangle\}\right]\times\mathcal{R}_{\ell,S,J}(r)=0. \quad (1)$$

Thus we seek an inversion scheme to specify two potential functions $V_c(r)$ and $V_{\rm so}(r)$. To do so requires knowledge of two sets of phase shifts. For spin-$\frac{1}{2}$ cases only two such sets exist having $J=L\pm\frac{1}{2}$. Only two sets would be required also if this approach was adopted to analyze the scattering of other (nonzero) spin particles. Choosing the cases $J=L\pm S$ means that the following development is extendable to all non-zero spin cases. For those two angular momentum sets, the Schrödinger equations reduce to the dimensionless forms

$$[(d^2/d\rho^2)+1-U_c(\rho)+SU_{\rm so}(\rho)\mp 2S\lambda U_{\rm so}(\rho)-(\lambda^2-\tfrac{1}{4})/\rho^2]\chi_\lambda^\pm(\rho)=0. \quad (2)$$

Therein, with $\lambda=\ell+0.5$, we have used $U_c(\rho)=V_c(r)/E$, $U_{\rm so}(\rho)=V_{\rm so}(r)/E$, $\rho=kr$, and $k=\sqrt{2\mu E/\hbar^2}$. Note that the spin value S only scales the spin-orbit potentials in these equations.

The global inverse scattering theory upon which our development is based is epitomized by the Sabatier interpolation formulas [4] by which the general Newton-Sabatier fixed energy inverse scattering theory [4] is approximated in a matrix form. The class of potentials resulting depends upon the nature of the selected indices (angular momentum values). The set corresponding to the physical angular momenta is a choice for which the phase shift function may be known from solely an analysis of scattering data. However, that may be too coarse a grid and a finer set can be chosen as the phase shift function can be specified at other angular momenta by analytic continuation. One could use Padé approximants to do that, but we find that a simple spline suffices. For the set of integer and half-integer values, however, Sabatier [10] generalized the matrix method specifically to give the interpolation formulas to effect inversion. The result is a set of equations from which the central and spin-orbit interactions can be specified by knowing at a fixed energy all of the phase shifts $\delta_\lambda^\pm$, at all positive integer and half-integer values of λ. Even so the inversion equations are nonlinear and so are very difficult to solve. The beauty of a method recently developed [9] is that the process can be transcribed to one of solving a set of linear-algebraic equations. The development given previously [9] is recast herein to allow any

value of spin S and to indicate advantages of different aspects in the technique of solution.

Suppose that $\psi_\lambda(r)$ and $\zeta_\lambda(r)$ are regular and irregular solutions (at the origin) of Schrödinger equations with a local central reference potential $U_{\rm ref}(r)$. The Sabatier interpolation formulas relate the regular solution of the complete problem, (2) to the set $\psi_\lambda(r)$ by

$$\chi_\lambda^\pm(\rho)=F^\pm(\rho)\psi_\lambda(\rho)+\sum_{\mu\in\Omega}\frac{2\mu}{\pi}W_{\lambda\mu}(\rho)\times[b_\mu\chi_\mu^\pm(\rho)-a_\mu^\pm\chi_\mu^\mp(\rho)], \tag{3}$$

wherein the Wronskian $W_{\lambda\mu}(\rho)=[\psi_\mu(\rho)\psi'_\lambda(\rho)-\psi_\lambda(\rho)\psi'_\mu(\rho)]/(\lambda^2-\mu^2)$ for the set of angular momenta Ω, $\{\frac{1}{2},1,\frac{3}{2},2,\frac{5}{2},3,\dots\}$, and the coefficients $a_\mu^\pm$ are to be found as part of the method of solution. The weights b_λ are 1 for integer λ and 0 otherwise for a zero reference potential. The scaling functions $F^\pm(\rho)$ are defined by

$$F^\pm(\rho)=(2/\pi\rho)\,a_0\chi_0(\rho)\psi_0(\rho)+\frac{2}{\pi\rho}\sum_{\mu\in\Omega}[a_\mu^\pm\chi_\mu^\mp(\rho)+b_\mu\chi_\mu^\pm(\rho)]\psi_\mu(\rho), \tag{4}$$

wherein $\chi_0(\rho)$ and $\psi_0(\rho)$ are solutions of the relevant Schrödinger equations for $\ell=-\frac{1}{2}$. When the scaling functions are known, the central and spin-orbit potentials follow from the identities [4]

$$U_{\rm so}=\pm(1/S\rho)\,(F^\pm)'/F^\pm \quad \text{with} \quad F^+F^-=1,$$
$$U_c=U_0+SU_{\rm so}-\frac{1}{\rho}(G^+F^-+G^-F^+)'+(\rho SU_{\rm so})^2, \tag{5}$$

in which we have used $G^\pm(\rho)=(2/\pi\rho)\Sigma_{\mu\in\Omega}\mu[a_\mu^\pm\chi_\mu^\mp(\rho)-b_\mu\chi_\mu^\pm(\rho)]\psi_\mu(\rho)$.

The inversion procedure involves two steps. First the potential coefficients $a_\lambda^\pm$ are ascertained from the chosen values of the phase shift set and the selected reference potential properties. In the second step we deduce the regular wave functions $\chi_\lambda^\pm(\rho)$. We then have all necessary ingredients to specify $U_c(\rho)$ and $U_{\rm so}(\rho)$.

The first step is achieved by considering the asymptotic properties of wave functions as they relate to the scattering phase shifts from data. Thus we assume that there is a radius ρ_0 beyond which we can take $U_{\rm so}(\rho)$ and $\Delta U(\rho)$ $[=U_c(\rho)-U_{\rm ref}(\rho)]$ both as zero. In that region, the exact solutions are simply linear combinations of the (known) regular and irregular solutions of the reference potential with phase shifts σ_λ, i.e.,

$$\chi_\lambda^\pm(\rho)=c_\lambda^\pm T_\lambda^\pm(\rho)=c_\lambda^\pm[\cos(\delta_\lambda^\pm-\sigma_\lambda)\psi_\lambda(\rho)+\sin(\delta_\lambda^\pm-\sigma_\lambda)\zeta_\lambda(\rho)]. \tag{6}$$

The scaling functions $F_\lambda^\pm$ reduce to the constants $h^\pm$, viz., $F^\pm(\rho>\rho_0)=h^\pm=\exp[\pm\int_0^{\rho_0}tSU_{\rm so}(t)dt]$.

Further we assume that the phase shift difference $\delta_\lambda^\pm-\sigma_\lambda$ vanishes for $\lambda\geqslant\lambda_{max}(\rho_0)$ so that the series can all be truncated to span the finite set Ω',$(\frac{1}{2},1,\frac{3}{2},\dots,\lambda_{max})$, and thus Eq. (3) equates to $4\lambda_{max}$ linear equations in the unknown coefficients, namely, for $\rho\geqslant\rho_0$ and $\lambda\in\Omega'$,

$$\psi_\lambda(\rho)=C_\lambda^\pm T_\lambda^\pm(\rho)+\sum_{\mu\in\Omega'}\frac{2\mu}{\pi}W_{\lambda\mu}(\rho)\times[T_\mu^\mp(\rho)A_\mu^\pm-b_\mu T_\mu^\pm(\rho)C_\mu^\pm]. \tag{7}$$

There are $8\lambda_{max}$ coefficients in all, viz,. $A_\lambda^\pm$ $(=a_\lambda^\pm c_\lambda^\mp h^\mp)$ and $C_\lambda^\pm$ $(=c_\lambda^\pm h^\mp)$. A solution can be formed by using information at two radial points ρ_0 and ρ_1 $(>\rho_0)$. $a_\lambda^\pm$ [now identified from $(h^\pm)^2A^\pm/C^\mp$] are ascertained when the $h^\pm$ are determined and those values follow from the $\lambda=0$ form for Eq. (7) as

$$(h^+)^2=\frac{\psi_0(\rho)+\sum_{\mu\in\Omega'}\frac{2\mu}{\pi}W_{0\mu}(\rho)[b_\mu T_\mu^-(\rho)C_\mu^--T_\mu^+(\rho)A_\mu^-]}{\psi_0(\rho)+\sum_{\mu\in\Omega'}\frac{2\mu}{\pi}W_{0\mu}(\rho)[b_\mu T_\mu^+(\rho)C_\mu^+-T_\mu^-(\rho)A_\mu^+]}. \tag{8}$$

The second step of the inversion process is to determine the inversion potentials. That requires evaluation of the solutions $\chi_\lambda^\pm(\rho)$ for all ρ. In the scheme we present that is done by multiplying Eq. (3) by $F^+(\rho)$ and rearranging to get a set of $8\lambda_{max}+1$ linear equations, viz.,

$$[F^+(\rho)]^2\psi_\lambda(\rho)=F^+(\rho)\chi_\lambda^+(\rho)-\sum_{\mu\in\Omega'}\frac{2\mu}{\pi}W_{\lambda\mu}(\rho)\times[b_\mu F^+(\rho)\chi_\mu^+(\rho)-a_\mu^+F^+(\rho)\chi_\mu^-(\rho)],$$

$$\psi_\lambda(\rho)=F^+(\rho)\chi_\lambda^-(\rho)-\sum_{\mu\in\Omega'}\frac{2\mu}{\pi}W_{\lambda\mu}(\rho)[b_\mu F^+(\rho)\chi_\mu^-(\rho)-a_\mu^-F^+(\rho)\chi_\mu^+(\rho)], \tag{9}$$

$$\{1-[F^+(\rho)]^2\}\psi_0(\rho)=\sum_{\mu\in\Omega'}\frac{2\mu}{\pi}W_{0\mu}(\rho)[(b_\mu+a_\mu^-)\times F^+(\rho)\chi_\mu^+(\rho)-(b_\mu+a_\mu^+)\times F^+(\rho)\chi_\mu^-(\rho)].$$

These equations can be solved for the $8\lambda_{max}+1$ values of $F^+(\rho)\chi_\lambda^\pm(\rho)$ and $F^+(\rho)$ at each value of $\rho\leqslant\rho_0$ desired. Thereafter $G^\pm(\rho)$ follow as do the inversion potentials from Eqs. (5).

This inversion process involves two ''technical parameters'' ρ_0 and ρ_1 $(=\rho_0+\Delta\rho)$. Our calculations have shown that the results are not sensitive to the exact choice of $\Delta\rho$, save that it should be small. However, the choice of the value of ρ_0 is critical. It must be large enough so that the asymptotic forms for the wave functions are valid but small enough so that the inversion method does not yield false (small-amplitude) oscillations in the potentials. The latter reflects a numerical problem when very large numbers of small phase shifts (even ones given with accuracy from the test potential calculation) must be used to find convergence of some series. Those large numbers of entries can dominate the matrix structure from which we have to specify the coefficients $a_\lambda^\pm$ such that false results are possible. The problem would be exacerbated if the process sought to start with actual data. The many small phase shift values for the large λ that are in the summations (λ_{max} is linked to ρ_0) then would be poorly known at best and many such small contributions add considerable uncertainties in results. We have also found that no advantage was gained by using more radial points ($\rho_i>\rho_0$) and thus seeking a solution of an overdetermined system of equations. In fact, our results were best always with just two radial points. However, the procedure so set was used as the benchmark for our improved scheme and we

designate it as the ''straightforward'' approach. We have found a way to improve the application of that straightforward method by reducing the reliance on the many partial terms to specify the scaling functions per Eq. (4). However, there is an even better way of proceeding, as we discuss next.

The problems described above are partly linked to the choice for the asymptotic behavior of the wave functions. Such wave functions are valid only for very large ρ $(\rightarrow\infty)$. A marked improvement has been found by using a technique developed by May *et al.* [11] with which the phase shifts are transformed so that one deals with new sets to be inverted using the scheme with no background. This development allows use of much smaller values of ρ_0 and λ_{max}. Essentially one assumes that the interaction is known at and beyond a reasonable matching radius as are the regular and irregular solutions of the Schrödinger equation of that (known) long-range potential form. The spin-orbit term is not affected by this process, so we consider just the central part in this discussion. We consider a potential

$$\tilde{V}(r)=\begin{cases} V_c(r) & \text{for } r<r_0 \ \ (=\rho_0/k) \\ V_c(r_0) & \text{for } r>r_0, \end{cases} \tag{10}$$

where $V_c(r_0)=2\eta E/\rho_0$ if the long-range potential is taken as the Coulomb interaction. If we consider the Schrödinger equation with the potential $\tilde{V}(r)-V_c(r_0)$, scattering phase shifts result by matching logarithmic derivatives at r_0 with the external solutions being free-particle (zero-potential) solutions. If the energy of such solutions is chosen to be $\tilde{E}=E-V_c(r_0)$, then the phase shifts so found $(\tilde{\delta}_\lambda)$ are linked to those for E and $V(r)$ by matching at $\rho=\rho_0$,

$$\begin{aligned}&[d/d(\beta\rho)]\ln[\cos\tilde{\delta}_\lambda H_\lambda(\beta\rho)+\sin\tilde{\delta}_\lambda I_\lambda(\beta\rho)] \\ &\quad=(1/\beta)\ (d/d\rho)\ln[\cos\delta_\lambda\psi_\lambda(\rho)+\sin\delta_\lambda\zeta_\lambda(\rho)],\end{aligned} \tag{11}$$

in which H_λ and I_λ are the regular and irregular free solutions (zero potential), respectively. The dimensionless ratio β is $\sqrt{1-V_c(\rho_0)/E}$ $(=\sqrt{1-2\eta/\rho_0}$ for the Coulomb potential). From Eq. (11), with the primes denoting differentiation with respect to $\beta\rho$, we deduce

$$\tilde{\delta}_\lambda=-\arctan\left(\frac{H'_\lambda(\beta\rho_0)-H_\lambda(\beta\rho_0)D_\lambda}{I'_\lambda(\beta\rho_0)-I_\lambda(\beta\rho_0)D_\lambda}\right), \tag{12}$$

where the right-hand side of Eq. (11) is denoted as D_λ. Inversion of the $\tilde{\delta}_\lambda$ gives a dimensionless potential $\tilde{U}(x)$ from which we obtain the full potential by the transforms $V_c(r)=E\ [\beta^2\tilde{U}(x)+1-\beta^2]$ and $r=x/k\beta$ for $r<r_0$.

As a test case of the method we consider the scattering of neutrons (spin $S=\frac{1}{2}$) from a potential of the Woods-Saxon form usually chosen as the (phenomenological) neutron-nucleus optical potential, namely,

$$\begin{aligned}V_c(r)&=-V_c\{1+\exp[(r-R)/a]\}^{-1}, \\ V_{\rm so}(r)&=2V_{\rm so}\frac{1}{r}\frac{d}{dr}\{1+\exp[(r-R)/a]\}^{-1}.\end{aligned} \tag{13}$$

The parameter values for the specific cases analyzed are $V_c=50$ MeV, $V_{\rm so}=15$ MeV, $R=3$ fm, and $a=0.6$ fm. The phase shift sets for this (purely real) interaction that we use in the first test of our scheme were evaluated at a center-of-mass energy of 150 MeV and a (free) wave number of 1.894 29 fm^{-1} (coinciding with a reduced mass of $m_n/2$).

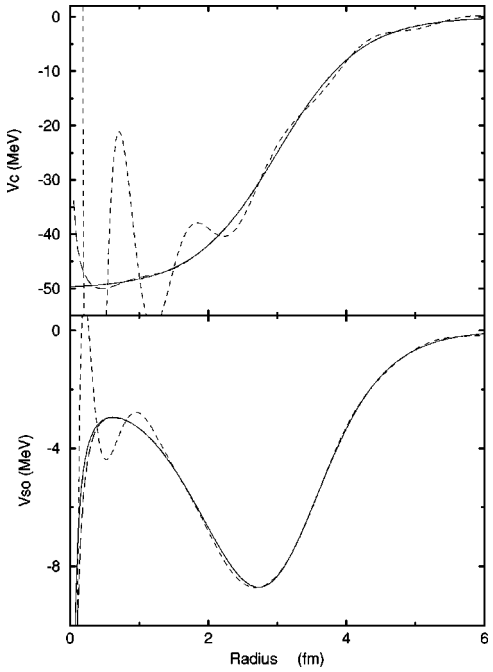

FIG. 1. Comparison of two inversion results with the original central $V_c(r)$ and spin-orbit $V_{\rm so}(r)$ potentials for scattering of 150-MeV neutrons. The original potentials are displayed by the solid curves, while the short- and long-dashed lines depict the inversion result found previously [9] and that found with our modified procedure, respectively.

Our first study was to invert those phase shifts using a zero background (reference) potential. This case is exactly that used in the study in [9]. The results are shown in Fig. 1, wherein the starting potentials are depicted by the solid curves and the results of the current inversion and of that found previously [9] are portrayed by the long- and short-dashed curves, respectively. Clearly our current result is markedly better as a reproduction of the starting interaction than the previous attempt. This is due to the way in which the scale functions $F^{\pm}(\rho)$ were calculated. In the previous study [9], Eq. (4) was used. For convergence, some 82 phase shift values were required $(\lambda_{max}=40)$ and the inversion potentials that result are sensitive to the exact choice of the many small values for the large λ. However, when we used Eq. (3) with $\lambda=0$ to obtain the scale functions, only 40 phase shifts in total were needed for convergence and the inversion potentials that result clearly reproduce the input interactions well.

This variant in the procedure has been used in the other studies we have made, first to add a Coulomb reference potential to the same real central plus spin-orbit interactions and then to allow the nuclear potentials to be complex. The results of those studies are shown in Figs. 2 and 3. We now consider the starting interaction to be representative of that for the scattering of two nuclei and so a point Coulomb interaction is included. That Coulomb interaction was set for a charge product Z_1Z_2 of 18, which gave a Sommerfeld parameter value of $\eta=0.163\,664$. Using the phase shift transform approach plus the method we now deem most useful to find the scaling functions, the inversion procedure leads to the results shown in Fig. 2. The matching radii ρ_0 and ρ_1 were taken as 19.8 and 19.81 fm and 40 partial waves only

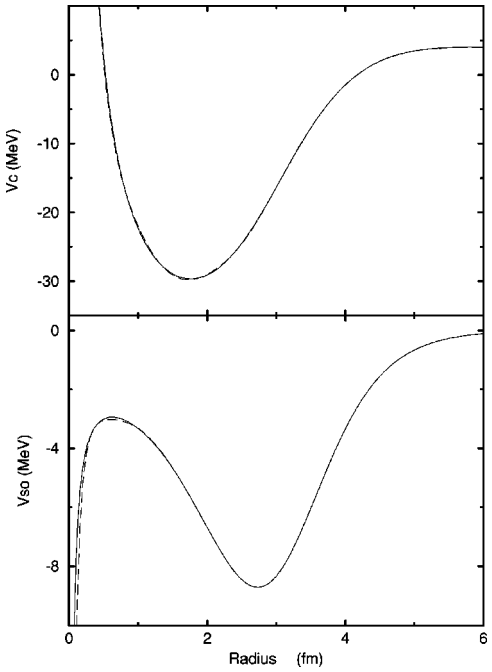

FIG. 2. Comparison of the inversion potentials with the original (nuclear) ones for a model nucleus-nucleus scattering problem in the case of $\eta = 0.163\,664$. The inversion procedure was made using a Coulomb background potential.

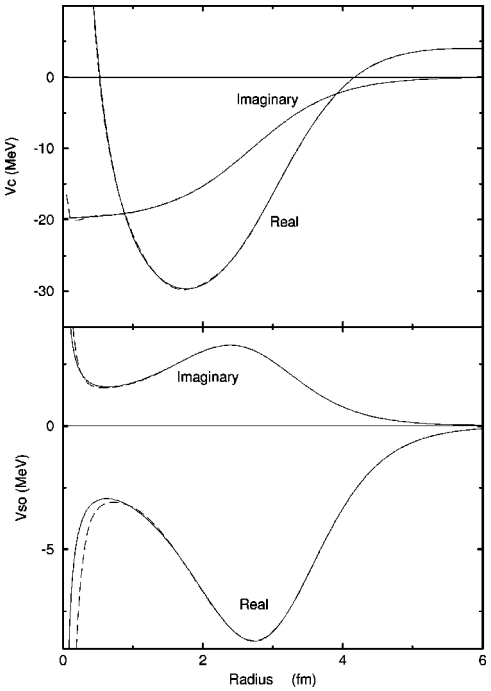

FIG. 3. Same as in Fig. 2 except for the addition of absorption in both the central and spin-orbit components.

are needed to give the results that are quite excellent reproductions of the starting potentials, even at quite small radii where the Coulomb field dominates.

There are cases where the potentials are complex, thereby allowing for scattering with a flux loss from the elastic channel. Our third application was to add to the preceding test interaction imaginary terms for both central and spin-orbit elements. The form of those imaginary potential terms is that given in Eq. (13), but with parameter values $V_c \Rightarrow W_c = 20$ MeV, $V_{so} \Rightarrow W_{so} = -7.5$ MeV, $R = 2.7$ fm, and $a = 0.6$ fm. The results of our inversion analyses are compared with the starting interactions in Fig. 3. The starting interactions are displayed by the solid curves, while the inversion results are shown by the dashed curves. The reproduction again is very good, but we do not do as well with the spin-orbit interaction for small radii $\leqslant 1$ fm. However, the short-range character of potentials does not greatly influence phase shift values and concomitantly are the least determined aspects in the inverse scattering theory.

In summary, the linear-algebraic reduction of the Sabatier interpolation formulas approach to inversion of scattering phase shifts from a central plus spin-orbit potential scattering problem works very well with sets of phase shifts typical for quantal scattering by potentials of short-range character. By using a phase shift transformation plus a reference background, it does so as well for interactions that have a long-range attribute, such as from a polarization potential with a $1/r^4$ asymptotic form in electron-atom scattering and from a Coulomb field in nuclear scattering. Complex phase shifts can also be used in the scheme to extract complex interactions that are typical for many atomic and nuclear scattering cases, although some loss in reproduction of details at small radii was found.

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