Eur. Phys. J. A **1**, 221–228 (1998)

THE EUROPEAN PHYSICAL JOURNAL A

An exact inversion method for the determination of spin–orbit potentials from scattering data

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Received: 30 April 1997 / Revised version: 20 October 1997
Communicated by W. Weise

Abstract. A generalized Newton–Sabatier inversion method which permits extraction from scattering data of central and spin-orbit potentials is presented. The inversion method originally developed by Sabatier and further elaborated by Hooshyar and Richardson, has been reformulated to lead to physically reasonable solutions and to allow for its numerical implementation. Numerical problems due to the occurrence of singularities in the transformation kernel are discussed and a successful application using schematic scattering data is reported.

PACS. 03.80.+r General theory of scattering – 24.90.+d Other topics in nuclear reactions: general – 25.40.-h Nucleon-induced reactions

1 Introduction

The solutions of inverse problems at fixed energy in quantum scattering theory provide efficient methods for the analyses of experimental scattering data. For more than three decades this topic has been studied quite intensively by mathematical physicists and today several mathematical formulations dealing with different types of interactions are available (see e.g. [1]). The inverse problem at fixed energy when only central interactions are involved is arguable the simplest and most studied one. For this case various inversion schemes, both quantal [2–4] and semiclassical [5], have been developed and applied successfully to experimental data.

The state of inverse scattering methods is less satisfactory for systems involving a spin–orbit interaction. Such systems are of particular interest in atomic and nuclear physics where the spin–orbit term is responsible for most of the level splitting and polarization phenomena. Including the spin–orbit operator in the inverse scattering problem requires the treatment of a coupled channel system where the interactions in various channels include potential terms linearly dependent on the orbital angular momentum quantum number ℓ. In contrast to the direct problem with spin–orbit potentials, there is no simple way of decoupling the equations in the inverse problem.

In the sixties, Sabatier [7] considered this type of inverse problems in some detail. Using the analytic properties of scattering wave functions, he constructed interpolation formulae of the Lagrange form which yield integral equations suitable for the coupled–channel inverse scattering problem at fixed energy with linearly ℓ-dependent potential terms. The original works [7] contain all the mathematical relations necessary to determine central and spin–orbit potentials knowing **S** matrix elements at integer and half integer values of ℓ. This method was extended by Hooshyar [8] and by Richardson and Hooshyar [9]. They reformulated the relevant equations and introduced an additional assumption about the required **S** matrix elements at "non-physical" half-integer values of ℓ, so that their method needs only **S** matrix elements at integer values of ℓ as input. Those values can be obtained from experiment, at least in principle. However, this inversion method still is rather involved. It has never been implemented numerically nor has it been applied to data analyses, either schematic or experimental data. Thus, to date, scattering data resulting from systems involving spin–orbit interactions have been analyzed by simulation, either by optical model fitting processes [8] or by the iterative perturbative method [10], both of which rely on iterative solutions of the direct problem. Recently, we developed an approximate inversion scheme with which it is possible to extract (approximate) central and spin–orbit interactions from the **S** matrix [11]. The method is based on a DWBA expansion in which the spin–orbit term is treated perturbatively and it has been applied successfully to analyze p-^{40}Ca elastic scattering data at intermediate energies [13].

In this paper we focus on the implementation of a quantum-mechanically exact inverse scattering solution for spin-$\frac{1}{2}$ channels involving spin–orbit potentials using the procedure as outlined by Sabatier [7] and Hooshyar [8] and present, using an adaption, the first application to realistic data. As mentioned above the mathematics given in the original papers [7,8] is rather involved and is not required in its full complexity to use the method as a tool. With such application in mind, we give a brief summary of the theory in section 2. For numerical implementation of the method specific questions must be considered care-

fully, and so in section 3, we discuss specifics of the determination of the potential coefficients via a generalization of the procedure of Münchow and Scheid [12] for the uncoupled equations. Other important topics dealt with in section 3 are the solution of the integral equation for the transformation kernel as well as the evaluation of the potentials via the associated differential equation. Numerically the latter exhibits unpleasant features. The feasibility of the method is demonstrated by a schematic example in section 4. Finally, in section 5 some concluding remarks are given.

2 The theory

We consider elastic scattering of a spin-$\frac{1}{2}$ particle by a potential that has central, $V_{\rm C}$, and spin–orbit, $V_{\rm SO}$, components. Using a partial wave expansion, the radial Schrödinger equation for the radial wave function $\psi^{(+)}_{j\ell}(E,r)$ takes the well known form

$$\left\{-\frac{\hbar^2}{2m}\left[\frac{d^2}{dr^2}-\frac{\ell(\ell+1)}{r^2}\right]+V_{\rm C}(r)+\langle\frac{\boldsymbol{s}\cdot\boldsymbol{l}}{\hbar^2}\rangle_{j\ell}V_{\rm SO}(r)\right\}$$
$$\times\psi^{(+)}_{j\ell}(E,r)=E\,\psi^{(+)}_{j\ell}(E,r), \qquad (1)$$

where E is the center of mass energy and j and ℓ are the total and orbital angular momentum quantum numbers, respectively. For spin-$\frac{1}{2}$ particles the expectation values of the spin–orbit operator is given by

$$2\langle\frac{\boldsymbol{s}\cdot\boldsymbol{l}}{\hbar^2}\rangle_{j\ell}=\begin{cases}\ell & \text{for} \quad j=\ell+\frac{1}{2}\\ -(\ell+1) & \text{for} \quad j=\ell-\frac{1}{2}\end{cases}. \qquad (2)$$

Following the general notation of inverse scattering theory we use $\lambda=\ell+\frac{1}{2}$ instead of ℓ because it leads to more convenient equations with regard to symmetry in λ. Furthermore, we eliminated the dimension of the equations substituting r by the variable $\rho=kr$ and defining the auxiliary potentials,

$$w_1(\rho)=\left[V_{\rm C}(\rho/k)-\frac{1}{4}V_{\rm SO}(\rho/k)\right]/E, \qquad (3)$$

$$w_2(\rho)=\frac{1}{4}V_{\rm SO}(\rho/k)/E. \qquad (4)$$

Thus the radial Schrödinger equation (1) is transformed into a system of equations,

$$\rho^2\frac{d^2}{d\rho^2}\psi^{\pm}_{\lambda}(\rho)+\rho^2\left[1-w_1(\rho)\mp 2\lambda w_2(\rho)\right]\psi^{\pm}_{\lambda}(\rho)$$
$$=(\lambda^2-\frac{1}{4})\psi^{\pm}_{\lambda}(\rho)\,, \qquad (5)$$

where the indices "$\pm$" refer to $j=\ell\pm\frac{1}{2}$, respectively.

Sabatier [7] and later Hooshyar [8] have studied extensively the properties of equation (5) by means of interpolation formulae. In the following we give a brief summary of their results which are essential to perform the inversion procedure. One important key for the solution of the inverse problem is the demonstration that the regular solution $\phi^{\pm}_{\lambda}(\rho)$ can be obtained from the regular solution $u_\lambda(\rho)$ of the potential free problem by the transformation

$$\phi^{\pm}_{\lambda}(\rho)=F^{\pm}(\rho)u_\lambda(\rho)-\int_0^\rho ds\,s^{-2}K^{\pm}_{\lambda}(\rho,s)u_\lambda(s), \qquad (6)$$

where $F^{\pm}(\rho)$ is directly related to the spin–orbit potential,

$$F^{\pm}(\rho)\;=\;\exp\left(\pm\int_0^\rho sw_2(s)ds\right). \qquad (7)$$

Similarly to inversion methods for uncoupled systems [2, 3] the integral kernels $K^{\pm}(\rho,\rho')$ represent a transformation kernel

$$\mathcal{K}(\rho,\rho')\;=\;\begin{pmatrix}K^{+}(\rho,\rho')\\ K^{-}(\rho,\rho')\end{pmatrix} \qquad (8)$$

which satisfies the integral equation

$$\mathcal{K}^T(\rho,\rho')=\mathcal{F}^T(\rho)\mathcal{E}(\rho,\rho')-\int_0^\rho ds\,s^{-2}\mathcal{K}^T(\rho,s)\mathcal{E}(s,\rho'). \qquad (9)$$

Here we have used the compact matrix notation as suggested by Hooshyar [8] where $\mathcal{F}(\rho)$ is defined by

$$\mathcal{F}(\rho)\;=\;\begin{pmatrix}F^{+}(\rho)\\ F^{-}(\rho)\end{pmatrix} \qquad (10)$$

and the upper index "T" denotes the transposition of the matrix. The matrix $\mathcal{E}(\rho,\rho')$ given by

$$\mathcal{E}(\rho,\rho')\;=\;\begin{pmatrix}-e(\rho,\rho') & q^{-}(\rho,\rho')\\ q^{+}(\rho,\rho') & -e(\rho,\rho')\end{pmatrix} \qquad (11)$$

is the input kernel of the inversion method and contains the spectral information via the potential coefficients $b^{\pm}_{\lambda}$ of the expansion of $q^{\pm}(\rho,\rho')$, viz.

$$q^{\pm}(\rho,\rho')\;=\;\sum_{\lambda\in\Omega}b^{\pm}_{\lambda}\,u_\lambda(\rho)u_\lambda(\rho')\,. \qquad (12)$$

The summation in equation (12) is given by the set, $\Omega=\left\{\frac{1}{2},\,1,\,\frac{3}{2},\,2,\,\ldots\right\}$, i.e. it extends over all positive integer and half integer values of λ. In analogy the function $e(\rho,\rho')$ is given by the expansion

$$e(\rho,\rho')\;=\;\sum_{\lambda\in\Omega}a_\lambda\,u_\lambda(\rho)u_\lambda(\rho')\,, \qquad (13)$$

where a_λ takes the values

$$a_\lambda=\begin{cases}2\lambda/\pi & \text{for} \quad \text{integer values of } \lambda\\ 0 & \text{for} \quad \text{half integer values of } \lambda\end{cases} \qquad (14)$$

for the specific case of vanishing reference potential $w_1^{(0)}=0$. At this point it should be emphasized that for a vanishing reference potential, the regular wave functions $u_\lambda(\rho)$ are the spherical Riccati–Bessel functions, $j_\lambda(\rho)$, for half integer values of λ and the cylindrical Riccati–Bessel functions for integer values of λ. For a more general consideration, the functions $u_\lambda(\rho)$ can be substituted by regular wave functions $u^{V_0}_{\lambda}(\rho)$ for a specific reference potential

$w_1^{(0)} = V_0$. These are associated with a modified set of a_λ and $b_\lambda^\pm$-values. In this paper, however, we restrict ourselves to $V_0 \equiv 0$.

In contrast to the case of uncoupled channels, the integral equation in the form of equation (9) does not allow a solution of the inverse problem. The difficulties are generated by the modification of the input kernel by the functions $F^\pm(\rho)$ which are unknowns of the inverse problem. Hooshyar [8] overcame these concerns by redefining the input kernel to be

$$\mathcal{G}(\rho,\rho') = f\,\mathcal{E}\,(\rho,\rho')\,f^{-1} \tag{15}$$

with

$$f = \begin{pmatrix} f_+ & 0 \\ 0 & f_- \end{pmatrix}, \tag{16}$$

where $f_\pm$ are given by

$$f_\pm = \lim_{\rho\to\infty} F^\pm(\rho). \tag{17}$$

This modified input kernel, $\mathcal{G}(\rho,\rho')$, is obtained by the expansion

$$\mathcal{G}(\rho,\rho') = \sum_{\lambda\in\Omega} u_\lambda(\rho)\,\mathcal{D}_\lambda\,u_\lambda(\rho') \tag{18}$$

where the coefficients $\mathcal{D}_\lambda$ are the 2×2 matrices

$$\mathcal{D}_\lambda \;=\; \begin{pmatrix} -a_\lambda & d_\lambda^- \\ d_\lambda^+ & -a_\lambda \end{pmatrix}. \tag{19}$$

The modified potential coefficients, $d_\lambda^\pm = f_\mp^2 b_\lambda^\pm$, can be obtained directly from the **S** matrix (see section 3.1) and therefore the kernel $G(\rho,\rho')$ can be determined. If one expresses the transformation kernel $\mathcal{K}(\rho,\rho')$ in terms of a matrix function $\mathcal{H}(\rho,\rho')$ defined by

$$\mathcal{K}(\rho,\rho') = \mathcal{F}(\rho) f^{-1}\,\mathcal{H}(\rho,\rho')\;f, \tag{20}$$

then one can rewrite the integral equation (9), in the familiar form

$$\mathcal{H}(\rho,\rho') \;=\; \mathcal{G}(\rho,\rho') - \int_0^\rho ds\, s^{-2}\mathcal{H}(\rho,s)\mathcal{G}(s,\rho')\,. \tag{21}$$

That equation is solvable for $\mathcal{H}(\rho,\rho')$.

Also in contrast to the case of uncoupled channels, the solution of equation (21) does not yield the transformation kernel from which the potential can be evaluated. A more sophisticated procedure is required [8]. It is based on the representation of the transformation kernel, $\mathcal{K}(\rho,\rho')$, in terms of the auxiliary potentials $w_1(\rho)$ and $w_2(\rho)$,

$$K^\pm(\rho,\rho) = \frac{1}{2}\rho F^\pm(\rho)\Big[\pm\rho^2 w_2(\rho) + \int_0^\rho ds\,(s^3 w_2^2(s) - s w_1(s))\Big], \tag{22}$$

which was derived by Sabatier [7]. From (22) it is straightforward to obtain the basic relations for the determination of the potentials, namely

$$\frac{2}{\rho^2}\left[F^-(\rho)K^+(\rho,\rho) - F^+(\rho)K^-(\rho,\rho)\right] = 2\rho w_2(\rho)\,, \tag{23}$$

$$\frac{1}{\rho}\;\left[F^-(\rho)K^+(\rho,\rho) + F^+(\rho)K^-(\rho,\rho)\right] = \int_0^\rho ds\,(s^3 w_2^2(s) - s w_1(s))\,. \tag{24}$$

Using the notation

$$\mathcal{H}(\rho,\rho') = \begin{pmatrix} H^{11}(\rho,\rho') & H^{12}(\rho,\rho') \\ H^{21}(\rho,\rho') & H^{22}(\rho,\rho') \end{pmatrix} \tag{25}$$

and

$$t(\rho) = \left(\frac{F^+(\rho)}{f^+}\right)^2 \tag{26}$$

one can write equation (23) as a differential equation, i.e.

$$\begin{aligned}\frac{d}{d\rho}t(\rho) \;&=\; \frac{2}{\rho^2}\left[H^{21}(\rho,\rho) - H^{12}(\rho,\rho)\,t^2(\rho)\right] \\ &+\; \frac{2}{\rho^2}\left[H^{11}(\rho,\rho) - H^{22}(\rho,\rho)\right]\,t(\rho)\,.\end{aligned} \tag{27}$$

Solving this equation with the boundary condition

$$\lim_{\rho\to\infty} t(\rho) = 1 \tag{28}$$

enables one to evaluate the auxiliary potentials by

$$w_2(\rho) \;=\; \frac{1}{2\rho}\frac{1}{t(\rho)}\frac{dt(\rho)}{d\rho}, \tag{29}$$

$$\begin{aligned} w_1(\rho) \;&=\; \rho^2 w_2^2(\rho) - \frac{1}{\rho}\frac{d}{d\rho} \\ &\times\; \left[\frac{1}{\rho}\left(H^{21}(\rho,\rho)\frac{1}{t(\rho)} + H^{12}(\rho,\rho)t(\rho)\right.\right. \\ &+\; \left.\left. H^{11}(\rho,\rho) + H^{22}(\rho,\rho)\right)\right], \end{aligned} \tag{30}$$

where (30) is a reformulation of (24). Thus the central and spin–orbit potentials are obtained directly via (3) and (4).

3 Implementation

3.1 Determination of the potential coefficients

The modified potential coefficients, $d_\lambda^\pm$, entering the input kernel, $\mathcal{G}(\rho,\rho')$, of the integral equation (21) contain the spectral information and must be determined from the phase shifts at integer and half integer values of the orbital angular momentum quantum number. For this purpose we consider (6) using the explicit expression for the transformation kernel,

$$\phi_\lambda^\pm(\rho) \;=\; F^\pm(\rho)u_\lambda(\rho) - \sum_{\mu\in\Omega}\left[\phi_\mu^\mp(\rho)b_\mu^\pm - \phi_\mu^\pm(\rho)a_\mu\right]L_{\mu\lambda}(\rho) \tag{31}$$

with

$$L_{\mu\lambda}(\rho) \;=\; \int_0^\rho ds\,s^{-2}\,u_\lambda(s)\,u_\mu(s)\,. \tag{32}$$

To derive a suitable relationship for the determination of the modified potential coefficients, $d_\lambda^\pm$, we define the function,

$$\chi_\lambda^\pm(\rho) \;=\; F^\mp(\rho)\,\phi_\lambda^\pm(\rho), \tag{33}$$

and rewrite (31) as

$$\chi_\lambda^\pm(\rho) \;=\; u_\lambda(\rho) - \sum_{\mu\in\Omega}\left[\chi_\mu^\mp(\rho) d_\mu^\pm \frac{1}{t(\rho)} - \chi_\mu^\pm(\rho) a_\mu\right] L_{\mu\lambda}(\rho)\,. \tag{34}$$

Because of the boundary condition on $t(\rho)$, (28), one can relate the modified potential coefficients, $d_\lambda^\pm$, to the asymptotic behaviour of $\chi_\lambda^\pm(\rho)$. For potentials of short range this yields the system of equations ($\lambda \in \Omega$)

$$B_\lambda^\pm e^{i\left(\delta_\lambda^\pm - \lambda\pi/2\right)} = e^{-i\pi\lambda/2} - \sum_{\mu\in\Omega}\left(B_\mu^\mp d_\mu^\pm\, e^{i\delta_\mu^\mp} - B_\mu^\pm a_\mu\, e^{i\delta_\mu^\pm}\right) \times\, e^{-i\pi\mu/2} L_{\mu\lambda}\,, \tag{35}$$

where $L_{\mu\lambda}$ is given by

$$L_{\mu\lambda} = \lim_{\rho\to\infty} L_{\mu\lambda}(\rho) = \frac{\sin\left((\lambda-\mu)\pi/2\right)}{\lambda^2-\mu^2}\left(1-\delta_{\mu\lambda}\right) + \frac{\pi}{4\lambda}\delta_{\mu\lambda}\,, \tag{36}$$

and $B_\lambda^\pm$ and $\delta_\lambda^\pm$ are the unknown asymptotic normalization of the wave functions and the (known) phase shifts, respectively.

The solution of (35) provides a set of $B_\lambda^\pm$ and $d_\lambda^\pm$ values for a given set of phase shifts, $\delta_\lambda^\pm$. This procedure is analogous to that for the determination of potential coefficients in the matrix method of Newton and Sabatier [3]. It yields unique potentials only with a further assumption concerning their asymptotic behaviour. An additional difficulty arises by the occurence of phase shifts at integer values of λ which cannot be extracted from experimental data at a given energy; a problem that Hooshyar overcame by the assumption $d_\lambda^\pm = a_\lambda$ at the "non-physical" λ-values. Choosing further the value of the potential coefficient $d_{1/2}^-$, he found a mathematically exact solution of the inverse problem. These assumptions, however, fix the phase shifts at integer λ-values in such a way that, in general, the associated potentials are not appropriate for use in physical applications.

In this paper we extend the procedure of Münchow and Scheid [12] to the case of spin-orbit potentials, by assuming that we know $w_1(\rho)$ and $w_2(\rho)$ for $\rho > \rho_0$. Thus one can determine the regular wave functions (apart from their normalizations) for $\rho > \rho_0$ from the knowledge of the phase shifts $\delta_\lambda^\pm$. If the potentials vanish for $\rho > \rho_0$, the regular wave functions in this domain are proportional to

$$T_\lambda^\pm(\rho) \;=\; \cos(\delta_\lambda^\pm) u_\lambda(\rho) - \sin(\delta_\lambda^\pm) v_\lambda(\rho)\,, \tag{37}$$

where $v_\lambda(\rho)$ are the Neumann functions for integer and half-integer values of λ. Substituting (37) into (34) yields the system of linear equations,

$$\sum_{\mu\in\Omega}\left\{\bar{B}_\mu^\pm\left[\delta_{\mu\lambda} - a_\mu\, L_{\mu\lambda}(\rho)\right] T_\mu^\pm(\rho) \;+\; \bar{d}_\mu^\pm L_{\mu\lambda}(\rho)\frac{1}{t(\rho)} T_\mu^\mp(\rho)\right\} = u_\lambda(\rho), \tag{38}$$

where $\bar{d}_\mu^\pm$ is defined by

$$\bar{d}_\mu^\pm \;=\; \bar{B}_\mu^\mp d_\mu^\pm\,. \tag{39}$$

In numerical calculations the sum in (38) must be restricted to a finite number of partial waves. Therefore we introduce the set $\bar{\Omega} = \{\frac{1}{2}, 1, \frac{3}{2}, \ldots, \lambda_{\max}\}$, where $\lambda_{\max}$ is the highest partial wave number taken into account. Using $\bar{\Omega}$ instead of Ω in (38) leads to a system of linear equations in $8\lambda_{\max}$ variables $\{\bar{d}_\mu^\pm, \bar{B}_\mu^\pm, \mu \in \Omega\}$. In principle (38) should be valid for all ρ–values with $\rho > \rho_0$. Hence, a system consisting of the equations at two ρ values $\rho_1, \rho_2 > \rho_0$ is solvable and leads to a unique set of potential coefficients $d_\lambda^\pm$ and normalization constants $\bar{B}_\lambda^\pm$.

As in the uncoupled case [12] the procedure does not yield potentials $w_1(\rho)$ and $w_2(\rho)$ with the prescribed behaviour for $\rho > \rho_0$. Rather it selects from the class of solutions of (21), the one which has the same relation of the regular wave functions at $\rho = \rho_1$ and $\rho = \rho_2$ and can be expressed by potential coefficients associated with the restricted set $\bar{\Omega}$. For a reliable inversion, therefore, it is of utmost importance to get an excellent description of the wave function in the vincinity of ρ_0 where the matching between the known and the unknown part of the potential occurs.

Taking into account this feature of the numerical procedure, we follow the suggestion of Münchow and Scheid [12] and consider the overdetermined system comprising the relations, (38), at several ρ-values ρ_k, $k = 1, 2, \ldots, N > 2$. The potential coefficients, $\bar{d}_\mu^\pm$, and normalization constants, $\bar{B}_\mu^\pm$, are then determined by minimizing the function

$$\chi^2 = \sum_{k=1}^{N}\sum_{\lambda\in\bar{\Omega}}\left\{\sum_{\mu\in\bar{\Omega}}\left[\left(\delta_{\mu\lambda} - a_\mu\, L_{\mu\lambda}(\rho_k)\right) T_\mu^\pm(\rho_k)\bar{B}_\mu^\pm + \frac{L_{\mu\lambda}(\rho_k)}{t(\rho_k)} T_\mu^\mp(\rho_k)\bar{d}_\mu^\pm\right] - u_\lambda(\rho_k)\right\}^2. \tag{40}$$

This minimization problem reduces to the solution of a system of linear equations and yields potentials which reproduce the regular wave functions at the ρ_k values. If the values ρ_k are chosen sufficiently near to ρ_0 it is reasonable to expect that the deviation of the inverted potentials from the prescribed one is minimal in the neighbourhood of ρ_0.

3.2 Solution of the integral equation

The central point of the inversion method, outlined in Sect. 2, is the solution of the integral (21) for all radii $\rho, \rho' < \rho_0$. The degenerate form of the modified input kernel $\mathcal{G}(\rho, \rho')$ implies a degenerate form of the modified transformation kernel $\mathcal{H}(\rho, \rho')$,

$$\mathcal{H}(\rho, \rho') = \sum_{\lambda\in\bar{\Omega}} Q_\lambda(\rho) u_\lambda(\rho')\,, \tag{41}$$

where the matrix valued function $Q_\lambda(\rho)$ can be obtained from the system of equations

$$\sum_{\mu\in\bar{\Omega}} Q_\lambda(\rho)\left[\delta_{\lambda\mu}\mathbf{1}+L_{\lambda\mu}(\rho)\right]=u_\lambda(\rho)D_\lambda,\quad \lambda\in\bar{\Omega}\,. \quad (42)$$

Thus the solution of the integral equation (21) reduces to an easily solvable algebraic problem.

To simplify the numerical implementation, as well as to reveal some algebraic features, we introduce the matrices

$$\mathbf{L}(\rho)=\begin{pmatrix} L_{\frac12\,\frac12}(\rho) & L_{\frac12\,1}(\rho) & \cdots & L_{\frac12\,\lambda_{\max}}(\rho)\\ L_{1\,\frac12}(\rho) & L_{1\,1}(\rho) & \cdots & L_{1\,\lambda_{\max}}(\rho)\\ \vdots & \vdots & \vdots & \vdots\\ L_{\lambda_{\max}\,\frac12}(\rho) & L_{\lambda_{\max}\,1}(\rho) & \cdots & L_{\lambda_{\max}\,\lambda_{\max}}(\rho)\end{pmatrix}, \quad (43)$$

$$\mathbf{D}^{ij}=\begin{pmatrix} D^{ij}_{\frac12} & 0 & \cdots & 0\\ 0 & D^{ij}_{1} & & \vdots\\ \vdots & & \ddots & 0\\ 0 & \cdots & 0 & D^{ij}_{\lambda_{\max}}\end{pmatrix} \quad (44)$$

and the vectors

$$Q^{ij}(\rho)=\begin{pmatrix} Q^{ij}_{\frac12}\\ \vdots\\ Q^{ij}_{\lambda_{\max}}\end{pmatrix}\quad\text{and}\quad u(\rho)=\begin{pmatrix} u_{\frac12}(\rho)\\ \vdots\\ u_{\lambda_{\max}}(\rho)\end{pmatrix}, \quad (45)$$

where ij refers to the matrix elements of the 2-dimensional matrices used before, $ij\in\{11,12,21,22\}$. The dimension of these vectors is equal to the number of elements of the set $\bar{\Omega}$. With this notation one can rewrite (42) and obtain the set of matrix equations,

$$\begin{aligned}
\left(\mathbf{1}+\mathbf{D}^{11}\,\mathbf{L}\right)Q^{11}+\mathbf{D}^{21}\,\mathbf{L}Q^{12}&=\mathbf{D}^{11}u\,,\\
\mathbf{D}^{12}\,\mathbf{L}Q^{11}+\left(\mathbf{1}+\mathbf{D}^{22}\,\mathbf{L}\right)Q^{12}&=\mathbf{D}^{12}u\,,\\
\left(\mathbf{1}+\mathbf{D}^{11}\,\mathbf{L}\right)Q^{21}+\mathbf{D}^{21}\,\mathbf{L}Q^{22}&=\mathbf{D}^{21}u\,,\\
\mathbf{D}^{12}\,\mathbf{L}Q^{21}+\left(\mathbf{1}+\mathbf{D}^{22}\,\mathbf{L}\right)Q^{22}&=\mathbf{D}^{22}u\,. \quad (46)
\end{aligned}$$

Using the equality of D^{11} and D^{22} (see (19)) we have derived the solution of (46) by standard algebraic manipulations. It can be written in the form

$$Q^{ij}(\rho)=M^{ij}(\rho)u(\rho)\,,\quad ij\in\{11,12,21,22\}\,, \quad (47)$$

where the matrices $M^{ij}(\rho)$ are given by

$$\begin{aligned}
\mathbf{M}^{11}(\rho)&=\mathbf{L}^{-1}\left\{\mathbf{L}+\left[\mathbf{D}^{21}(\mathbf{L}^{-1}+\mathbf{D}^{11})^{-1}\mathbf{D}^{12}\right.\right.\\
&\quad\left.\left.-\ (\mathbf{L}^{-1}+\mathbf{D}^{11})\right]^{-1}\right\}\mathbf{L}^{-1}\,,\\
\mathbf{M}^{12}(\rho)&=-\mathbf{L}^{-1}\left(\mathbf{L}^{-1}+\mathbf{D}^{11}\right)^{-1}\mathbf{D}^{12}\\
&\quad\times\left[\mathbf{D}^{21}(\mathbf{L}^{-1}+\mathbf{D}^{11})^{-1}\mathbf{D}^{12}-(\mathbf{L}^{-1}+\mathbf{D}^{11})\right]^{-1}\mathbf{L}^{-1},\\
\mathbf{M}^{21}(\rho)&=-\mathbf{L}^{-1}\left(\mathbf{L}^{-1}+\mathbf{D}^{11}\right)^{-1}\mathbf{D}^{21}\\
&\quad\times\left[\mathbf{D}^{12}(\mathbf{L}^{-1}+\mathbf{D}^{11})^{-1}\mathbf{D}^{21}-(\mathbf{L}^{-1}+\mathbf{D}^{11})\right]^{-1}\mathbf{L}^{-1},\\
\mathbf{M}^{22}(\rho)&=\mathbf{L}^{-1}\left\{\mathbf{L}+\left[\mathbf{D}^{12}(\mathbf{L}^{-1}+\mathbf{D}^{11})^{-1}\mathbf{D}^{21}\right.\right.\\
&\quad\left.\left.-\ (\mathbf{L}^{-1}+\mathbf{D}^{11})\right]^{-1}\right\}\mathbf{L}^{-1}\,. \quad (48)
\end{aligned}$$

The matrix elements of the transformation kernel are then obtained by the compact form

$$\mathcal{H}^{ij}(\rho,\rho')=u^T(\rho')\mathbf{M}^{ij}(\rho)u(\rho)\,. \quad (49)$$

This representation of the transformation kernel is very convenient for a numerical implementation because all matrices involved are either symmetric ($\mathbf{L}=\mathbf{L}^T$) or diagonal ($\mathbf{D}^{11},\mathbf{D}^{12},\mathbf{D}^{21},\mathbf{D}^{22}$). A consequence of this symmetry is the relation

$$\mathbf{M}^{11}=\left(\mathbf{M}^{22}\right)^T \quad (50)$$

which can easily be seen from (48). It is obvious that this feature simplifies the solution of the integral equation considerably and reduce the computing time of numerical codes. For the solution of the inverse problem we need the values of the transformation kernels $\mathcal{H}^{ij}$ at $\rho=\rho'$ only. At this specific argument, the representation given in (49) exhibits similar features as the trace. In particular, using the relation (50) we obtain the identity

$$H^{11}(\rho,\rho)=H^{22}(\rho,\rho), \quad (51)$$

which simplifies the differential equation (27) for the determination of the potential.

3.3 Determination of the potentials

The scattering potentials are finally obtained via (3), (4), (29) and (30) from the solution of the differential equation (27), i.e. of

$$\frac{dt}{d\rho}=\frac{2}{\rho^2}\left[H^{21}(\rho,\rho)-H^{12}(\rho,\rho)\,t^2\right]\,, \quad (52)$$

with the boundary condition given by (28), and with use of the identity in (51). In general the numerical solution of a first order differential equation is straightforward. However, there arise severe problems in the solution of (52) because both $H^{21}(\rho,\rho)$ and $H^{12}(\rho,\rho)$ exhibit several singularities as a function of ρ. Analysis of the properties of (48) shows that these singularities must occur in both kernels at the same radii $\rho_s, s=1,2,\ldots$. Thus to solve (52) we have developed a specific procedure based on spline and optimization techniques. Considering (52) at a point ρ_s with singular transformation kernels one can easily derive the corresponding t-value, namely

$$t(\rho_s)=\lim_{\rho\to\rho_s}\sqrt{\frac{H^{21}(\rho_s,\rho_s)}{H^{12}(\rho_s,\rho_s)}}\,. \quad (53)$$

We exploit this fact and define a coarse mesh comprising the singularities $(\rho_s,\,t(\rho_s))$, $s=1,2,\ldots$ and the boundary condition $(\rho_\infty,1)$ where ρ_∞ is a sufficient large radius. Performing a spline interpolation through these mesh points provides a first estimate of the solution $t(\rho)$. In a further step we redefine the procedure and define additional mesh points at radii between the singularities using the corresponding values as a variable in a subsequent optimization procedure. These variables are adjusted in such a way that the corresponding spline interpolation best satisfies (52).

Table 1. The potential coefficients $d_\lambda^\pm$ for the test case

λ	d_λ^+	d_λ^-	λ	d_λ^+	d_λ^+
0.5	0.75037E+02	-0.24503E+00	9.5	-0.12369E+06	-0.29836E+06
1.0	-0.42304E+03	0.62296E+01	10.0	0.80942E+04	0.38599E+06
1.5	0.13529E+04	-0.50300E+02	10.5	0.14033E+06	-0.17238E+06
2.0	-0.30899E+04	0.18083E+03	11.0	-0.10447E+06	0.39657E+04
2.5	0.30177E+04	-0.43150E+03	11.5	-0.21687E+05	-0.56898E+05
3.0	0.38417E+03	-0.99403E+02	12.0	0.37251E+05	0.55644E+05
3.5	-0.66170E+04	0.28642E+04	12.5	0.67948E+04	0.20556E+06
4.0	0.75944E+04	-0.57466E+04	13.0	0.44840E+05	-0.46232E+06
4.5	0.73857E+04	-0.11274E+05	13.5	-0.12828E+06	0.41877E+06
5.0	-0.32569E+05	0.10356E+06	14.0	0.11183E+06	-0.18300E+06
5.5	0.36210E+05	-0.41408E+06	14.5	-0.48527E+05	-0.35183E+05
6.0	0.68139E+04	0.21477E+06	15.0	-0.27800E+04	0.21630E+06
6.5	-0.57161E+05	-0.88386E+06	15.5	0.10040E+06	-0.27987E+06
7.0	0.21360E+05	0.10766E+07	16.0	-0.17332E+06	0.84170E+05
7.5	0.12953E+06	-0.83267E+06	16.5	0.73778E+05	0.17460E+06
8.0	-0.26089E+06	0.30821E+06	17.0	0.75405E+05	-0.15016E+06
8.5	0.20115E+06	0.70865E+05	17.5	-0.69682E+05	-0.64422E+05
9.0	0.11566E+05	-0.34048E+04	18.0	0.22353E+05	0.11913E+06

Thus we obtain an excellent approximation of the function $t(\rho)$.

One can even improve the method by the use of a numerical filter smoothing the resulting function $t(\rho)$. Thus one can eliminate numerical inaccuracies in the transformation kernels, $H^{12}(\rho,\rho)$ and $H^{21}(\rho,\rho)$, which are always present in the vicinity of singularities.

4 Example

The present inversion method has been developed with regard to its numerical implementation. It is therefore of utmost interest to demonstrate the feasibility of the method by application to a realistic example.

We consider a neutron scattered off a nucleus at a laboratory energy $E_{\rm lab} = 100$ MeV. In our example we neglect the recoil of the target and assume a realistic neutron-nucleus interaction consisting of a central part,

$$V_{\rm C}(r) = -V_0^{\rm C}\,\left[1+\exp(\frac{r-R}{a})\right]^{-1}, \qquad (54)$$

and a spin-orbit part

$$V_{\rm SO}(r) = V_0^{\rm SO}\,\frac{1}{r}\frac{d}{dr}\,\left[1+\exp(\frac{r-R}{a})\right]^{-1}. \qquad (55)$$

The parameters are fixed to the values

$$V_0^{\rm C} = 50 \text{ MeV},\ V_0^{\rm SO} = 5 \text{ MeV},\ R = 3.42 \text{ fm},\ a = 0.50 \text{ fm}. \qquad (56)$$

which represent a reasonable choice for a typical neutron-nucleus potential.

With this potential in the Schrödinger equations, we evaluated the phase shifts at integer and half integer values of the angular momentum at $E_{\rm lab} = 100$ MeV. These phase shifts are displayed in Fig. 1 and show clearly their continuous behaviour as a function of ℓ. They have been used as input quantities for the inversion procedure; the goal of which is to reconstruct the schematic potential, equations (54-56). To apply the inversion procedure, it is necessary to evaluate the potential coefficients $d_\lambda^\pm$ in the first step. For this purpose we fix the highest partial

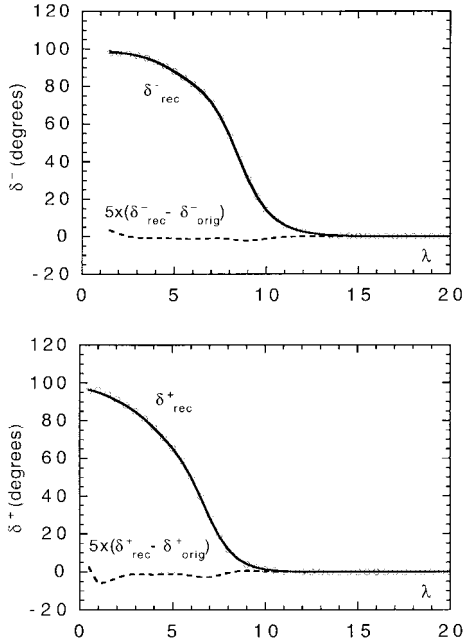

Fig. 1. The λ-dependence of the scattering phase shifts for the model example discussed in the text. The *circles* indicate the values $\delta_{\rm orig}$ which are used as input in the inversion procedure. The *solid curves* show the phase shifts $\delta_{\rm rec}$ evaluated with the reconstructed potential. The *dashed curves* give the difference of the evaluated phase shifts

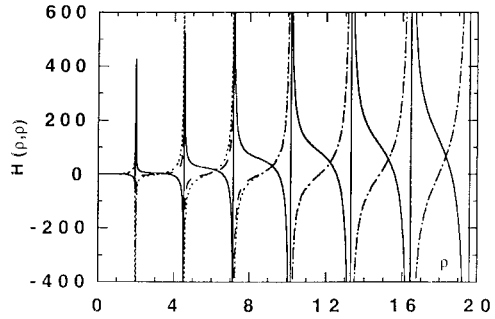

Fig. 2. The matrix elements of the transformation kernel as a function of ρ for the example discussed in the text. The *solid line* is $H^{11}(\rho,\rho)$, the *dashed line* is $H^{12}(\rho,\rho)$ and the *dotted line* is $H^{21}(\rho,\rho)$. At larger values the *dashed* and the *dotted values* are on top of each other

wave $\lambda_{\max} = 18$ included in the set $\bar{\Omega}$ and the matching point $\rho_0 = 20$. These technical parameters have been the best choice for the considered example and in Table 1 we present the numerical values of the potential coefficients. Similarly to values found using the Newton-Sabatier method there is usually no convergence of the potential coefficients visible at the numerically considered values of λ.

In principle the potential coefficients $\bar{d}^{\pm}_{\lambda}, \lambda \in \bar{\Omega}$ reflect the spectral information and can be used to determine the modified input kernel $\mathcal{G}(\rho,\rho')$ for the integral (21). Within our algorithm outlined in Sect. 3.2 this is not necessary; it suffices to construct the matrices $\mathbf{D}^{12}$ and $\mathbf{D}^{21}$. The matrix elements of the transformation kernel $H^{12}(\rho,\rho)$, $H^{21}(\rho,\rho)$ and $H^{11}(\rho,\rho) = H^{22}(\rho,\rho)$ are then obtained by straightforward calculation via equations (48) and (49) and are displayed in Fig. 2. As mentioned previously the functions $H^{12}(\rho,\rho)$, $H^{21}(\rho,\rho)$, and $H^{11}(\rho,\rho)$ exhibit singularities at several ρ values. For all three matrix elements, these singularities occur at the same ρ-values because they are generalized by zero points of the determinant of the same operator.

The solution of the differential equation (52) yielding the basis function $t(\rho)$ for the determination of the potentials is tedious because of the singularities of $H^{12}(\rho,\rho)$ and $H^{21}(\rho,\rho)$. For the application of our procedure (Subsect. 3.3) the ratio $\sqrt{H^{21}/H^{12}}$ must be well defined in the vicinity of the singularity. That this is indeed the case is shown in Fig. 3 at two specific singularities. Despite the obviously large numerical errors of $H^{12}(\rho,\rho)$ and $H^{21}(\rho,\rho)$ in the neighbourhood of a singularity, the ratio $\sqrt{H^{21}/H^{12}}$ at singularities is well defined and gives a reasonable estimate of the function $t(\rho)$. Hence, these values can be used in the subsequent optimization procedure for $t(\rho)$.

The final step in the process is to evaluate the potentials V_{C} and V_{SO} from $t(\rho)$. In Fig. 4 the inverted potentials are compared with the original ones. For both potential contributions we obtain an excellent reconstruction for $r > 1$ fm. At smaller radii the inversion potentials exhibit similar deficiencies to those of central potentials obtained by the Newton-Sabatier method (cf. [12]). This is not surprising because we have limited the expansion

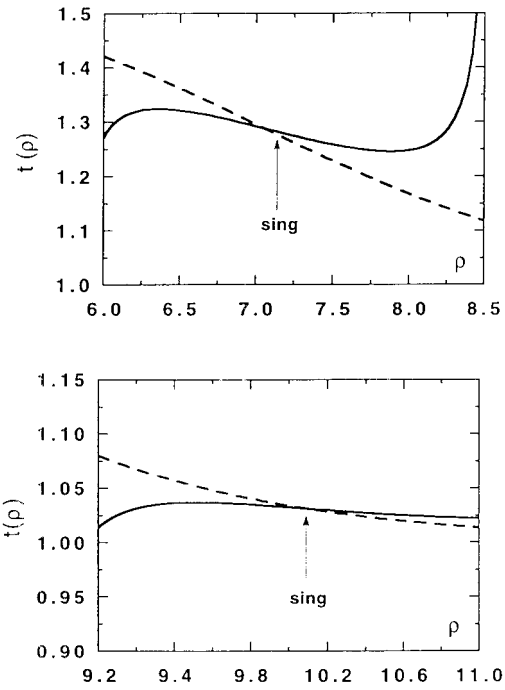

Fig. 3. The functional behaviour of the ratio $\sqrt{H^{21}(\rho,\rho)/H^{12}(\rho,\rho)}$ in the vicinity of the singularities at $\rho_s = 7.14$, $\rho_s = 10.10$ (*solid line*). For comparison we show the function $t(\rho)$ (*dashed lines*) as obtained directly from the model spin–orbit potential. The *arrows* indicate the position of the singularities

of the modified input kernel to a finite number of partial waves.

The quality of the inversion procedure can also be demonstrated by the evaluation of the phase shifts using the reconstructed potential in the Schrödinger equation. As can be seen from Fig. 1 the deviations of the reevaluated phase shifts from the original ones are smaller than 0.4 degree except for $\lambda = 0.5$ and 1.5, where the differences reach 1 degree.

5 Summary

We have reformulated the inversion method, originally derived by Sabatier [7] and further developed by Hooshyar [8], to make it suitable for numerical implementation. That reformulation facilitates determination of quantum mechanically exact central and spin-orbit potentials via inversion techniques from scattering data. The method can be considered as a generalized Newton–Sabatier inversion procedure. This becomes most evident in the determination of potential coefficients reflecting the spectral information, and like the standard Newton–Sabatier method these potential coefficients are not defined uniquely. To find uniqueness then, we have generalized the method of Münchow and Scheid [12] which selects the potential out of the class of exact solutions of the integral equation that reproduces best the behaviour of the regular wave functions in the vicinity of the matching point. But as this

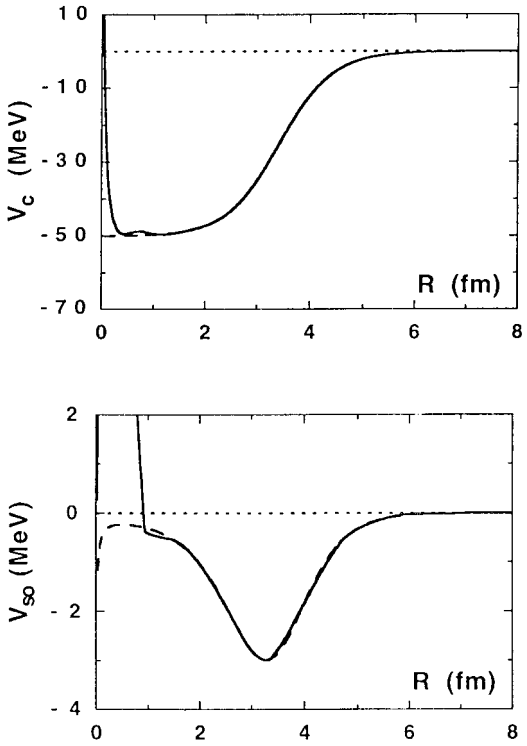

Fig. 4. Comparison of the inverted potentials (*solid line*) with the original ones (*dashed line*) for the model example of neutron–nucleus scattering that is discussed in the text. The central and spin-orbit potentials are shown in the top and bottom respectively

is only an approximate inversion, the result will depend slightly on the technical parameter ρ_0. However, our numerical example indicates that the method provides sufficiently accurate inversion results.

The presented inversion procedure requires knowledge of the phase shifts at integer and half–integer values of λ. While the phase shifts at half–integer values are used in the equations of the elastic cross section at the given energy, there is no such relationship to observables involving the phase shifts at integer values of λ. There is some hope that reliable values of the phase shifts at integer λ-values can be extracted by analyzing the observables at neighbouring energies; the assumption being that the phase shifts are continous function of E and λ. However, an algorithm to provide this information is not available as yet. A further point which must be considered with regard to application, is the extension of the procedure to deal with complex potentials.

This research was supported by the Jubiläumsfond der Österreichischen Nationalbank, project Nr. 4537. The authors are indepted to Prof. Dr. K. Amos for fruitful discussions as well as reading the manuscript.

References

1. Chadan, K., Sabatier, P. C.: Inverse Problems in Quantum Scattering Theory, Berlin, Heidelberg, New York: Springer 1989
2. Burdet, G., Giffon, M., Predazzi, E.: Nuovo Cimento **36**, 1337 (1965), ibid. **44A**, 138 (1966)
3. Newton, R.G.: J. Math. Phys., **3**(1), 75 (1961); Sabatier P C, J. Math. Phys. **7**, 1515 (1966), ibid. **7**, 2079 (1966), ibid. **8**, 905 (1967)
4. Lipperheide, R., Fiedeldey, H.: Z. Phys. A **286**, 45 (1978), ibid. A **301**, 81 (1981)
5. Kujawski, E.: Phys. Rev. C **6**, 709 (1972).
6. Hodgson, P.E.: The Optical Model of Elastic Scattering, Oxford: Claredon Press, 1963; Varner, R.L., Thomson, W.J., Mc Abee, T.L., Ludwig, E.J., Clegg, T.B.: Phys. Rep. C **201**, 57 (1991)
7. Sabatier, P.C.: J. Math. Phys. **7**, 1515 (1966), ibid. **9**, 1241 (1968), ibid. **13**, 675 (1972)
8. Hooshyar, M.A.: J. Math. Phys. **12**, 2243 (1971), ibid. **16**, 257 (1975), ibid. **19**, 253 (1978), ibid. **32**, 2310 (1991)
9. Richardson, P.A., Hooshyar, M.A.: J. Math. Phys. **32** (5), 1310 (1991)
10. Ioannides, A.A., Mackintosh, R.S.: Nucl. Phys. A **467**, 482 (1987)
11. Leeb, H., Huber, H., Fiedeldey H.: Phys. Lett. B **344**, 18 (1995)
12. Münchow, M., Scheid, W.: Phys. Rev. Lett. **44**, 1299 (1980)
13. Huber, H., Leeb, H.: Application of global inversion techniques to proton-nucleus scattering data, preprint IK-TUW-Preprint 9606401: TU Wien, 1996