# Solution of a Coupled Channel Inverse Scattering Problem at Fixed Energy by a Modified Newton-Sabatier Method

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The modified Newton-Sabatier method is extended to the inverse scattering problem of coupled channels at fixed energy. The problem is solved for a system of coupled radial Schrödinger equations with a potential matrix independent of the angular momentum of the relative motion. The new method is applied to the example of two channels coupled by complex-valued square well potentials. [S0031-9007(96)01001-0]

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The inverse scattering problem in quantum mechanics plays an important role in the determination of effective potentials from measured cross sections. The fixed angular momentum problem for one channel can be solved by the Gel'fand-Levitan method [1] or by the Marchenko method [2]. An extension of the Gel'fand-Levitan method to coupled channels was developed by Cox [3]. A rational scheme was proposed by Kohlhoff and von Geramb [4] and applied to nucleon-alpha spin-orbit interactions by Becker [5].

The fixed energy inversion problem was solved for one channel by Newton [6] and Sabatier [7]. Reviews are given in Refs. [8] and [9]. Münchow and Scheid [10] modified the one channel Newton-Sabatier method under the assumption that the spherical potential $V(r)$ is known from a certain finite distance $r_0$ up to infinity, which is usually the case in practice. With this modification the method is applicable to realistic heavy ion collisions [11,12]. A spin-orbit inversion scheme at fixed energy was given by Leeb *et al.* [13] and applied by Alexander *et al.* [14] to derive nucleon-alpha spin-orbit potentials. The results of these calculations compare well to the potentials obtained by Becker [5]. In this Letter we extend the modified Newton-Sabatier method to the case of $N$ coupled channels under the assumption that the potential matrix does not depend on the angular momentum of relative motion.

*The coupled channel equations.*—We assume that the Hamiltonian of two colliding partners (nuclei or atoms) can be written in the form $H = T(\mathbf{r}) + h(\xi) + W(r,\xi)$, where $T$ denotes the relative kinetic energy operator, $h$ the Hamiltonian of the internal states of the two scattering partners with internal excitation energies $\epsilon_\alpha$ ($\epsilon_1 = 0 < \epsilon_2 \leq \cdots \leq \epsilon_N$), and $W$ the interaction energy depending on the set of internal coordinates $\xi$ and the relative radial distance $r$. Then the wave function of the scattering problem $H\psi = E\psi$ can be expanded as

$$\Psi_{\ell m} = \sum_{\alpha=1}^{N}\sum_{n=1}^{N} R_{\alpha n}^{\ell}(r)\chi_\alpha(\xi)Y_{\ell m}(\hat{r})\,. \qquad (1)$$

Here $Y_{\ell m}$ describes the orbital motion of the nuclei or atoms with the angular momentum quantum numbers $\ell$ and $m$, $\alpha$ denotes the channel number, and $n$ enumerates the $N$ degenerate solutions belonging to the same given energy $E$.

Projecting $(H - E)\Psi_{\ell m} = 0$ with the channel states, one obtains the following coupled equations for the radial functions:

$$\left[-\frac{\hbar^2}{2\mu}\,\frac{1}{r}\,\frac{d^2}{dr^2}r + \frac{\hbar^2}{2\mu}\,\frac{\ell(\ell+1)}{r^2} + \epsilon_\alpha - E\right]R_{\alpha n}^{\ell}(r) + \sum_{\beta=1}^{N} V_{\alpha\beta}(r)R_{\beta n}^{\ell}(r) = 0\,, \qquad (2)$$

where $V_{\alpha\beta}(r) = \langle\chi_\alpha|W|\chi_\beta\rangle$ is the potential matrix. Using dimensionless coordinates we rewrite Eq. (2) in the form

$$\sum_{\beta=1}^{N} D_{\alpha\beta}^{U}(\rho)\varphi_{\beta n}^{\ell}(\rho) = \ell(\ell+1)\varphi_{\alpha n}^{\ell}(\rho) \qquad (3)$$

with

$$D_{\alpha\beta}^{U}(\rho) = \rho^2\left\{\left[\frac{d^2}{d\rho^2} + \frac{E_\alpha}{E}\right]\delta_{\alpha\beta} - U_{\alpha\beta}(\rho)\right\}, \qquad (4)$$

where the following abbreviations have been introduced: $\rho = kr$, $k = (2\mu E)^{1/2}/\hbar$, $E_\alpha = E - \epsilon_\alpha$, $\varphi_{\alpha n}^{\ell}(\rho) = \rho R_{\alpha n}^{\ell}(r)$, and $U_{\alpha\beta}(\rho) = V_{\alpha\beta}(r)/E$.

We next choose an arbitrary symmetric matrix $U_{\alpha\beta}^{0}(\rho) = U_{\beta\alpha}^{0}(\rho)$ for the reference potential whose regular solutions $\varphi_{\alpha n}^{0\ell}$ of the Schrödinger equation are known:

$$\sum_{\beta=1}^{N} D_{\alpha\beta}^{U_0}(\rho)\varphi_{\beta n}^{0\ell}(\rho) = \ell(\ell+1)\varphi_{\alpha n}^{0\ell}(\rho) \qquad (5)$$

with

$$D_{\alpha\beta}^{U_0}(\rho) = \rho^2\left\{\left[\frac{d^2}{d\rho^2} + \frac{E_\alpha}{E}\right]\delta_{\alpha\beta} - U_{\alpha\beta}^{0}(\rho)\right\}. \qquad (6)$$

The potential matrix $U_{\alpha\beta}$ is the unknown quantity which we determine from given $S$-matrix elements $S_{\alpha\beta}^{\ell}$ of the radial wave functions $\varphi_{\alpha n}^{\ell}$.

  

*The inverse problem for coupled channels at fixed energy.*—Let us generalize the Povzner-Levitan representation of the scattering solution functions for the case of $N$ coupled channels as

$$\varphi^{\ell}_{\alpha n}(\rho) = \varphi^{0\ell}_{\alpha n}(\rho) - \sum_{\beta=1}^{N} \int_0^{\rho} \frac{d\rho'}{\rho'^2} K^{UU_0}_{\alpha\beta}(\rho,\rho')\varphi^{0\ell}_{\beta n}(\rho'), \tag{7}$$

where the matrix elements $K^{UU_0}_{\alpha\beta}$ of the transformation kernel will be specified later. It is a straightforward exercise to show that the solution functions $\varphi^{\ell}_{\alpha n}$, as expressed in Eq. (7), satisfy the coupled radial Schrödinger equations (3), if use of Eq. (5) and of the following relations is made:

$$\sum_{\beta=1}^{N} D^{U}_{\alpha\beta}(\rho)K^{UU_0}_{\beta\gamma}(\rho,\rho') = \sum_{\beta=1}^{N} D^{U_0}_{\gamma\beta}(\rho')K^{UU_0}_{\alpha\beta}(\rho,\rho'), \tag{8}$$

$$U_{\alpha\beta}(\rho) = U^0_{\alpha\beta}(\rho) - \frac{2}{\rho}\frac{d}{d\rho}\frac{K^{UU_0}_{\alpha\beta}(\rho,\rho)}{\rho}. \tag{9}$$

The latter equation yields the wanted potential. The transformation kernel is the solution of the partial differential equation (8), which is equivalent to the integral equation of Gel'fand-Levitan type as given in Ref. [9].

It is easy to prove that the following transformation kernel matrix fulfills Eq. (8):

$$K^{UU_0}_{\alpha\beta}(\rho,\rho') = \sum_{\ell=0}^{\infty}\sum_{n=1}^{N}\sum_{n'=1}^{N} c^{\ell}_{nn'}\varphi^{\ell}_{\alpha n}(\rho)\varphi^{0\ell}_{\beta n'}(\rho'). \tag{10}$$

Inserting this equation into Eq. (7), we get the fundamental equations for the inverse calculation of the coupled channel problem:

$$\varphi^{\ell}_{\alpha n}(\rho) = \varphi^{0\ell}_{\alpha n}(\rho) - \sum_{\ell'=0}^{\infty}\sum_{n'=1}^{N}\sum_{n''=1}^{N} \varphi^{\ell'}_{\alpha n'}(\rho)c^{\ell'}_{n'n''}L^{\ell'\ell}_{n''n}(\rho), \tag{11}$$

where the matrix $\mathbf{L}$ is given as

$$L^{\ell\ell'}_{nn'}(\rho) = \sum_{\alpha=1}^{N}\int_0^{\rho} \frac{d\rho'}{\rho'^2}\varphi^{0\ell}_{\alpha n}(\rho')\varphi^{0\ell'}_{\alpha n'}(\rho'). \tag{12}$$

Solving Eq. (11) for the spectral coefficients $c^{\ell}_{nn'}$ and the radial functions $\varphi^{\ell}_{\alpha n}(\rho)$, we obtain the coupling potentials by use of Eqs. (9) and (10).

*The usual Newton-Sabatier method.*—The spectral coefficients $c^{\ell}_{nn'}$ can be obtained as a function of the $S$ matrix by analyzing Eq. (11) in the limit $\rho \to \infty$. Let us assume that the asymptotic wave functions are connected with the $S$ matrices as follows $[\rho \to \infty, \kappa_\alpha = (E_\alpha/E)^{1/2}]$:

$$\varphi^{\ell}_{\alpha n}(\rho) = \sum_{n'=1}^{N} \rho T^{\ell}_{\alpha n'}(\rho)A^{\ell}_{n'n} \tag{13}$$

with

$$T^{\ell}_{\alpha n}(\rho) = (e^{-i(\kappa_\alpha\rho-\ell\pi/2)}\delta_{\alpha n} - S^{\ell}_{\alpha n}e^{i(\kappa_\alpha\rho-\ell\pi/2)})/(\kappa_\alpha\rho), \tag{14}$$

$$\varphi^{0\ell}_{\alpha n}(\rho) = (e^{-i(\kappa_\alpha\rho-\ell\pi/2)}\delta_{\alpha n} - S^{0\ell}_{\alpha n}e^{i(\kappa_\alpha\rho-\ell\pi/2)})/\kappa_\alpha. \tag{15}$$

The $S$-matrix elements $S^{\ell}_{\alpha n}$ are the input data for the calculation; the elements $S^{0\ell}_{\alpha n}$ are known and belong to the reference potential $U^0_{\alpha\beta}$. The coefficients $A^{\ell}_{nn'}$ serve as normalization and expansion coefficients of the solution functions. Inserting Eqs. (13) and (15) into Eq. (11) we get incoming and outgoing waves on both sides of Eq. (11). Thus we can write (11) in terms of $\exp(i\kappa_\alpha\rho)$ and $\exp(-i\kappa_\alpha\rho)$. To fulfill this equation, the coefficients of the exponential functions must vanish. By setting them to zero, we get a set of equations for $c^{\ell}_{nn'}$ and $A^{\ell}_{nn'}$, which are linear in $A^{\ell}_{nn'}$ and $b^{\ell}_{nn'} = \sum_{n''=1}^{N} A^{\ell}_{nn''}c^{\ell}_{n''n'}$. After eliminating the coefficients $A^{\ell}_{nn'}$, we can calculate the coefficients $b^{\ell}_{nn'}$:

$$b_\mu = \sum_\nu M^{-1}_{\mu\nu}N_\nu \quad [\mu = (\ell,\alpha,n), \nu = (\ell',n',n'')], \tag{16}$$

where $M_{\mu\nu} = (S^{\ell}_{\alpha n'}e^{i(\ell'-\ell)/2} - S^{\ell'}_{\alpha n'}e^{i(\ell-\ell')\pi/2})L^{\ell'\ell}_{n''n}(\infty)$ and $N_\mu = S^{\ell}_{\alpha n} - S^{0\ell}_{\alpha n}$. We then find

$$c^{\ell}_{nn'} = \sum_{n''=1}^{N}(A^{\ell})^{-1}_{nn''}b^{\ell}_{n''n'}, \tag{17}$$

$$A^{\ell}_{nn'} = \delta_{nn'} - \sum_{\ell'=0}^{\infty}\sum_{n''=1}^{N} e^{i(\ell'-\ell)\pi/2}b^{\ell'}_{nn''}L^{\ell'\ell}_{n''n'}(\infty). \tag{18}$$

Since the number of channels $N$ is finite for each angular momentum, the proof of the uniqueness of the resulting coupling matrix $U_{\alpha\beta}$ can be carried out in the same manner as in the case of $N = 1$ [7]. If we consider the special case $U^0_{\alpha\beta} = 0$ with $S^{0\ell}_{\alpha n} = \delta_{\alpha n}$, we can generalize the proof of Sabatier [7] that one (and only one) potential of the form (9) with (10) exists if the matrix elements $S^{\ell}_{\alpha n} - \delta_{\alpha n}$ drop faster than $\ell^{-3-\epsilon}$ for $\ell \to \infty$. Then the potential matrix $U_{\alpha\beta}$ goes to zero faster than $\rho^{-2+\epsilon}$ as $\rho \to \infty$, whereas all the equivalent coupling potentials are damped out [7]. Therefore we assume that the above inversion method yields a unique result for $U_{\alpha\beta}$ if $U_{\alpha\beta}$ vanishes faster than $\rho^{-2+\epsilon}$ as $\rho \to \infty$.

*The modified Newton-Sabatier method.*—In many applications the coupling potential is known from some radius $r_0$ on. As an example, let us assume in the following that the interaction is zero beyond a particular radius $r_0$ in all channels:

$$U_{\alpha\beta}(\rho) = 0, \qquad \rho \geq \rho_0 = kr_0. \tag{19}$$

Then the information, inherent in the $S$ matrix, is used to construct the coupling matrix only in the finite interval of $0 < r < r_0$. This is the purpose of the modified Newton-Sabatier method, which has been shown to yield unique potentials of the form (9) with (10) [10].

Because of (19), it is suitable to choose a zero reference potential: $U^0_{\alpha\beta} \equiv 0$. Then the regular reference solutions are taken as $\varphi^{0\ell}_{\alpha n}(\rho) = \rho T^{0\ell}_{\alpha n}(\rho)$

with $T^{0\ell}_{\alpha n}(\rho) \equiv \delta_{\alpha n} j_\ell(\kappa_\alpha \rho)$. Inserting these functions and $\varphi^\ell_{\alpha n}(\rho)$ of Eq. (13) into Eq. (11) and limiting the number of $\ell$ values to $\ell_{\max}$, we get the following finite set of coupled equations:

$$\sum_{n'=1}^{N} \left( T^\ell_{an'}(\rho) A^\ell_{n'n} + \sum_{\ell'=0}^{\ell_{\max}} T^{\ell'}_{\alpha n'}(\rho) b^{\ell'}_{n'n} L^{\ell'\ell}_n(\rho) \right) = T^{0\ell}_{\alpha n}(\rho) \tag{20}$$

with $L^{\ell\ell'}_n(\rho) = \int_0^\rho j_\ell(\kappa_n \rho') j_{\ell'}(\kappa_n \rho')\, d\rho'$. The coefficients $A^\ell_{nn'}$ and $b^\ell_{nn'}$ are obtained by solving Eq. (20) at outer radii $\rho_i > \rho_0$, where $T^\ell_{\alpha n}(\rho)$ is determined by the given $S$ matrix: $T^\ell_{\alpha n}(\rho > \rho_0) = \delta_{\alpha n} h^-_\ell(\kappa_\alpha \rho) - S^\ell_{\alpha n} h^+_\ell(\kappa_\alpha \rho)$ with $h^\pm_\ell(x) = j_\ell(x) \pm i n_\ell(x)$. Choosing two radii $\rho_1, \rho_2 > \rho_0$ we get a set of $2 \times (\ell_{\max} + 1) \times N \times N$ equations for the unknown coefficients $A^\ell_{nn'}$ and $b^\ell_{nn'}$. Then the use of Eq. (11) at various values of $\rho < \rho_0$ together with Eqs. (9) and (10) gives the inverted potential matrix. As the coefficients depend weakly on $\rho_1$ and $\rho_2$, one can apply a least-squares method in order to find an optimum solution of Eq. (20) at $M$ least-squares points $\rho_1, \rho_2, \ldots, \rho_M (\rho_i > \rho_0)$ [10]. Equation (20) yields a unique solution for $A^\ell_{nn'}$ and $b^\ell_{nn'}$ and then also for the potential matrix $U_{\alpha\beta}$ for $\ell_{\max} \to \infty$, independent of $\rho_i > \rho_0$. This can be proven by the same methods as used for $N = 1$ [10]. In practice, the values of $\ell_{\max}$ are restricted by the numerical precision in solving Eq. (20) and, therefore, a minor dependence of $U_{\alpha\beta}$ on $\ell_{\max}$ and $\rho_i > \rho_0$ results.

*Application.*—We applied our method to the case of two coupled square well potentials. For this problem, analytic solutions for the $S$ matrix were derived by Lovas [15], which we used in our calculation. As an example, we set the potential matrix (in MeV) as

$$\mathbf{V}(r) = \begin{cases} \begin{pmatrix} -6 - 4i & -5 \\ -5 & -4 - 2i \end{pmatrix} & \text{for } r \leq 6 \text{ fm}, \\ 0 & \text{for } r > 6 \text{ fm}. \end{cases} \tag{21}$$

Here the real part describes the attraction of the scattering partners and the imaginary part models the absorption from the considered channels. The excitation energies were set $\epsilon_1 = 0$ MeV and $\epsilon_2 = 5$ MeV. The mass parameter was chosen as the reduced mass for the scattering of two alpha particles.

In Fig. 1 the results of the inversion calculations at different scattering energies are shown. With increasing energy, the number of usable $S$–matrix elements raises with angular momentum, containing more information about the potential matrix. The higher the energy, the higher $\ell_{\max}$ can be chosen in Eq. (20). The energy was set $E = 7$ MeV ($\ell_{\max} = 8$), 10 MeV ($\ell_{\max} = 9$), and 50 MeV ($\ell_{\max} = 17$) for the dotted, dashed, and full curves, respectively. In order to have a quantitative comparison of these calculations, a $\chi^2$ test has been performed. The $\chi^2$ error function was defined as

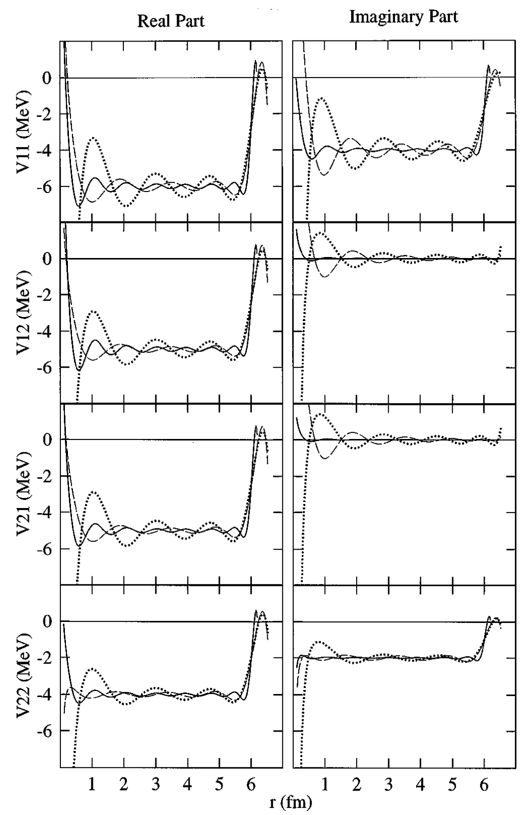


FIG. 1. The potential matrix elements $V_{\alpha\beta}$ inverted at $E = 7$, 10, and 50 MeV (cm energy) are shown as a function of the radial distance by dotted, dashed, and full curves, respectively. The chosen radii are $r_1 = 6.18$ fm and $r_2 = 6.22$ fm.

$$\chi^2 = \frac{1}{N} \sum_{i=1}^{N} \sum_{\alpha=1}^{2} \sum_{\beta=1}^{2} \left| \frac{V^{\text{cal}}_{\alpha\beta} - V^{\text{exact}}_{\alpha\beta}}{1 \text{ MeV}} \right|^2 . \tag{22}$$

The $\chi^2$ values for the potentials are $\chi^2 = 3.2224$, 1.3458, and 0.5074 for $E = 7$, 10, and 50 MeV, respectively.

The potentials in Fig. 1 show small oscillations around the exact potential values with an approximate wavelength $\lambda \approx 0.25 h/(2\mu E)^{1/2}$ and amplitudes which get smaller as more angular momenta are taken into account in Eq. (20). The wavelength arises from the variations of the product terms $\varphi^\ell_{\alpha n} \varphi^{0\ell}_{\beta n'}$ in the kernel (10). We note that the inverted potential matrix has a pole for $r = 0$ as can be seen from Eq. (9).

In conclusion, for the first time the Newton-Sabatier method is extended to a special coupled channel problem. The coupling potential is restricted to monopole transitions induced by the radial motion. The extension of the method to charged scattering partners is straightforward by applying the procedure of May *et al.* [11]. A comparison with experimental data is presently difficult since in practice nuclei or atoms are scattered with initial ground state configurations and, therefore, only a row of the $S$ matrix is experimentally known. An extended paper with details of the method will be presented in the near future.

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