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Coupled channel inverse scattering problem at fixed energy in Born approximation

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Abstract
An approximative method based on the first Born approximation is developed for the solution of the quantum inverse scattering problem at fixed energy for coupled reaction channels. The method allows us to obtain the local coupling matrix from the S-matrix. It is applied to cases with given monopole and dipole couplings in order to test the quality of the couplings resulting from the inversion of the S-matrix.

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1. Introduction

The quantum inverse scattering method is concerned with finding the potentials from the knowledge of differential cross sections [1, 2]. In principle we can distinguish two types of inversion methods, at fixed energy and at fixed angular momentum. Most inversion methods treat only the inverse elastic scattering problem and are able to calculate the potential from elastic scattering phase shifts. The inversion at fixed angular momentum is based on the theory of Gel'fand and Levitan [3]. It was extended to coupled reaction problems [4] by using Marchenko equations [5] and applied to experimental data in [6].

For the elastic inverse problem at fixed energy, several methods are known in the literature to obtain the potential from the phase shifts, namely the inversion methods of Newton and Sabatier [7, 8], with Bargman potentials [9], the method of finite differences [10] and the method using the WKB approximation [11]. Only the modified Newton–Sabatier method [8] was extended to reaction channels coupled with a monopole-type interaction [12] and further approximately expanded to dipole and quadrupole interactions [13]. No other inversion method is known to us to solve the inelastic quantum inverse problem at fixed energy, i.e. the problem of extracting the coupling potentials from the knowledge of the complete S-matrix at fixed energy.

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In this paper, we present an approximative treatment of the solution of the inelastic inverse scattering problem at fixed energy by starting from the S-matrix. This method is an extension of the approximative method of Ramm [14–16] for the solution of the elastic inverse problem. The approximation applied there is the same as used in the first Born approximation and allows us to write the moments of the potentials as functions of the phase shifts. These moments can be inverted to the potential with the method of Backus and Gilbert [17, 18]. The applicability and limits of Ramm's inverse scattering method are the same as for the Born approximation.

In section 2, we express the S-matrix of the coupled channel problem at fixed energy by an integral over the product of the coupling potentials and the coupled radial wavefunctions. These connecting equations are approximated in section 3 by replacing the exact wavefunctions by free solutions as in the first Born approximation. Then we obtain moments of the coupling potentials as functions of the S-matrix which are resolved by the method of Backus and Gilbert. For a practical proof and test of the new method, we consider cases with monopole and dipole couplings in section 4. Finally in section 5 we give a summary and conclusions and an estimate of the quality of inversion in the appendix.

2. The coupled channel problem

In order to apply the inversion method of [14] to the scattering of a projectile with a target, we first formulate the Hamiltonian of the coupled channel problem. As usual we make the following ansatz for the Hamiltonian [13]:

$$\hat{H}(\mathbf{r},\xi) = \hat{T}(\mathbf{r}) + \hat{h}(\xi) + \hat{W}(\mathbf{r},\xi), \tag{1}$$

where $\hat{T}(\mathbf{r})$ is the kinetic energy operator of the relative motion, $\hat{h}(\xi)$ is the Hamiltonian for the excitation of the internal degrees of freedom of the scattered particles, described by the set of internal coordinates ξ, and $\hat{W}(\mathbf{r},\xi)$ is the interaction energy coupling the intrinsic and relative dynamics of the particles. The internal Hamiltonian has the eigenvalues $\varepsilon_{\nu J}$ and the eigenfunctions $\chi_{\nu JM}(\xi)$:

$$\hat{h}(\xi)\chi_{\nu JM}(\xi) = \varepsilon_{\nu J}\chi_{\nu JM}(\xi). \tag{2}$$

Here, ν is a quantum number, J is the total intrinsic angular momentum and M is its projection. The interaction potential is short-ranged up to $r \leqslant a$ and is expanded in a spherical representation:

$$\hat{W}(\mathbf{r},\xi) = \sum_{\lambda=0}^{\infty}\sum_{\mu=-\lambda}^{\lambda} Q_{\lambda\mu}(r,\xi)Y^{*}_{\lambda\mu}(\Omega). \tag{3}$$

The stationary solution of the coupled channel problem $\hat{H}\Psi = E\Psi$ can be written as

$$\Psi^{I}_{M}(\mathbf{r},\xi) = \sum_{\nu,J}\sum_{\ell=|I-J|}^{I+J} R^{I}_{\nu J\ell,n}(r)[\mathrm{i}^{\ell}Y_{\ell}(\Omega)\otimes\chi_{\nu J}(\xi)]^{I}_{M}, \tag{4}$$

where $\otimes$ denotes the tensor product of the spherical harmonics $Y_{\ell m}(\Omega)$ and the internal wavefunctions $\chi_{\nu JM}(\xi)$, coupled to the conserved quantum numbers I and M of the total angular momentum and its projection, respectively. We assume that K intrinsic channels are coupled defined by the set of quantum numbers (ν, J). The index n denotes the N linearly independent physical solutions of the N coupled differential equations for the radial functions $R^{I}_{\nu J\ell,n}(r)$ for fixed I with

$$N = \sum_{(\nu,J)=1}^{K} \min(2I+1, 2J+1). \tag{5}$$

In the following we use the symbol α for the set of quantum numbers $\alpha = (\nu_\alpha, J_\alpha, \ell_\alpha)$. Inserting the wavefunction (4) into the eigenvalue equation and projecting with channel states, we obtain coupled differential equations for the radial wavefunctions [13]:

$$\left(\frac{1}{r}\frac{\mathrm{d}^2}{\mathrm{d}r^2}r - \frac{\ell_\alpha(\ell_\alpha+1)}{r^2} + k_\alpha^2\right) R^I_{\alpha n}(r) = \sum_\beta U^I_{\alpha\beta}(r) R^I_{\beta n}(r) \tag{6}$$

with $k_\alpha^2 = \frac{2\mu}{\hbar^2}\left(E - \varepsilon_{\nu_\alpha J_\alpha}\right)$ and

$$U^I_{\alpha\beta}(r) = \frac{2\mu}{\hbar^2}\sum_\lambda \mathrm{i}^{\ell_\beta-\ell_\alpha}(-1)^{I+J_\alpha+\lambda}\frac{1}{\sqrt{4\pi}}\sqrt{(2\ell_\alpha+1)(2\lambda+1)(2\ell_\beta+1)} \times \begin{Bmatrix} \ell_\alpha & \lambda & \ell_\beta \\ J_\beta & I & J_\alpha \end{Bmatrix} \begin{pmatrix} \ell_\alpha & \lambda & \ell_\beta \\ 0 & 0 & 0 \end{pmatrix} \langle \nu_\alpha J_\alpha \| Q_\lambda \| \nu_\beta J_\beta \rangle, \tag{7}$$

where μ is the reduced mass in the relative motion and $\langle \nu_\alpha J_\alpha \| Q_\lambda \| \nu_\beta J_\beta \rangle$ is the reduced matrix element of the multipole interaction $Q_{\lambda\mu}$ with respect to the intrinsic states. The coupled differential equations (6) can be transformed to coupled integral equations:

$$R^I_{\alpha n}(r) = R^{0I}_{\alpha n}(r) - \mathrm{i}\int_0^a r'^2\,\mathrm{d}r' k_\alpha j_{\ell_\alpha}(k_\alpha r_<) h^{(1)}_{\ell_\alpha}(k_\alpha r_>) \sum_\beta U^I_{\alpha\beta}(r') R^I_{\beta n}(r'). \tag{8}$$

Here, $R^{0I}_{\alpha n}(r)$ are regular, so-called free solutions of the uncoupled differential equations

$$\left(\frac{1}{r}\frac{\mathrm{d}^2}{\mathrm{d}r^2}r - \frac{\ell_\alpha(\ell_\alpha+1)}{r^2} + k_\alpha^2\right) R^{0I}_{\alpha n}(r) = 0, \tag{9}$$

and the functions $h^{(1)}_\ell$ are the complex sum of the regular and irregular spherical Bessel functions: $h^{(1)}_\ell = j_\ell + \mathrm{i}n_\ell$. The symbols $r_<$ and $r_>$ in (8) denote the smaller and larger values of r and r', respectively.

Next we assume short-range potentials $U^I_{\alpha\beta}(r)$ which vanish after a radial distance a. Then we can write the wavefunctions $R^I_{\alpha n}(r)$ for $r > a$:

$$R^I_{\alpha n}(r > a) = C^I_{\alpha n} j_{\ell_\alpha}(k_\alpha r) - \mathrm{i} I^I_{\alpha n}\left(j_{\ell_\alpha}(k_\alpha r) + \mathrm{i}n_{\ell_\alpha}(k_\alpha r)\right) \tag{10}$$

with the interaction matrix

$$I^I_{\alpha n} = \int_0^a r'^2\,\mathrm{d}r' k_\alpha j_{\ell_\alpha}(k_\alpha r') \sum_\beta U^I_{\alpha\beta}(r') R^I_{\beta n}(r'). \tag{11}$$

The constants $C^I_{\alpha n}$ can be freely chosen. We set them $C^I_{\alpha n} = \delta^I_{\alpha,n=\beta}$. Then the wavefunctions (10) can be expressed in terms of the S-matrix:

$$R^I_{\alpha\beta}(r > a) = \tfrac{1}{2}\left(\left(S^I_{\alpha\beta} + \delta^I_{\alpha\beta}\right) j_{\ell_\alpha}(k_\alpha r) + \mathrm{i}\left(S^I_{\alpha\beta} - \delta^I_{\alpha\beta}\right) n_{\ell_\alpha}(k_\alpha r)\right) \tag{12}$$

with

$$\begin{aligned} S^I_{\alpha\beta} &= \delta^I_{\alpha\beta} - 2\mathrm{i} I^I_{\alpha\beta}, \\ \delta^I_{\alpha\beta} &= \delta_{\nu_\alpha\nu_\beta}\delta_{J_\alpha J_\beta}\delta_{\ell_\alpha\ell_\beta}\Delta(J_\alpha\ell_\alpha I)\Delta(J_\beta\ell_\beta I). \end{aligned} \tag{13}$$

The quantity $\Delta(J\ell I)$ has the values $\Delta = 1$ if the quantum numbers J, ℓ and I fulfil the triangle condition and $\Delta = 0$ otherwise.

3. The inversion method

For solving the inversion problem we apply the method of Ramm [14] which is tested for the one-channel case, i.e. the elastic scattering [15, 16]. According to this method, we approximate the interaction matrix (11) by the first Born approximation, replacing the exact solution $R^I_{\beta n}(r)$ by the free solution $R^{0I}_{\beta n}(r) = \delta^I_{\beta n} j_{\ell_\beta}(k_\beta r)$:

$$I^I_{\alpha\beta} \to \tilde{I}^I_{\alpha\beta} = \int_0^a r'^2 \,\mathrm{d}r' k_\alpha j_{\ell_\alpha}(k_\alpha r') U^I_{\alpha\beta}(r') j_{\ell_\beta}(k_\beta r'). \tag{14}$$

This leads to the basic equation of our inversion procedure:

$$S^I_{\alpha\beta} - \delta^I_{\alpha\beta} = -2\mathrm{i}\tilde{I}^I_{\alpha\beta}. \tag{15}$$

3.1. Resolution for moments of transition matrix

Now we intend to extract the intrinsic diagonal and transition potentials $\langle \nu_\alpha J_\alpha \| Q_\lambda \| \nu_\beta J_\beta \rangle$ from equation (15). To isolate the moments of these potentials we carry out a sum over the angular momentum quantum number I. Inserting $\tilde{I}^I_{\alpha\beta}$ of (14) and $U^I_{\alpha\beta}$ of (7) into (15), and multiplying both sides with a $6j$-symbol we obtain

$$\begin{aligned}\sum_I (-1)^I (2I+1)(2\lambda'+1) \begin{Bmatrix} J_\beta & \ell_\beta & I \\ \ell_\alpha & J_\alpha & \lambda' \end{Bmatrix} \left(S^I_{\alpha\beta} - \delta^I_{\alpha\beta}\right) \\ = -\frac{4\mathrm{i}\mu k_\alpha}{\hbar^2} \mathrm{i}^{\ell_\beta - \ell_\alpha} (-1)^{-J_\alpha} \frac{1}{\sqrt{4\pi}} \sqrt{(2\ell_\alpha+1)(2\ell_\beta+1)} \int_0^a r'^2 \,\mathrm{d}r' j_{\ell_\alpha}(k_\alpha r') j_{\ell_\beta}(k_\beta r') \\ \times \sum_\lambda (-1)^\lambda \sqrt{2\lambda+1} \begin{pmatrix} \ell_\alpha & \lambda & \ell_\beta \\ 0 & 0 & 0 \end{pmatrix} \langle \nu_\alpha J_\alpha \| Q_\lambda \| \nu_\beta J_\beta \rangle \\ \times \sum_I (2I+1)(2\lambda'+1) \begin{Bmatrix} J_\beta & \ell_\beta & I \\ \ell_\alpha & J_\alpha & \lambda' \end{Bmatrix} \begin{Bmatrix} \ell_\alpha & \ell_\beta & \lambda \\ J_\beta & J_\alpha & I \end{Bmatrix}. \end{aligned} \tag{16}$$

Because the last sum over I is $\delta_{\lambda\lambda'}$ [19], we find

$$\int_0^a r'^2 \,\mathrm{d}r' j_{\ell_\alpha}(k_\alpha r') j_{\ell_\beta}(k_\beta r') \langle \nu_\alpha J_\alpha \| Q_\lambda(r', \xi) \| \nu_\beta J_\beta \rangle = b^\lambda_{\alpha\beta} \tag{17}$$

where $b^\lambda_{\alpha\beta}$ is given by

$$\begin{aligned} b^\lambda_{\alpha\beta} = \frac{\mathrm{i}\hbar^2\sqrt{4\pi}}{4\mu k_\alpha} \mathrm{i}^{\ell_\alpha - \ell_\beta} (-1)^{J_\alpha + \lambda} \sqrt{\frac{2\lambda+1}{(2\ell_\alpha+1)(2\ell_\beta+1)}} \begin{pmatrix} \ell_\alpha & \lambda & \ell_\beta \\ 0 & 0 & 0 \end{pmatrix}^{-1} \\ \times \sum_I (-1)^I (2I+1) \begin{Bmatrix} J_\beta & \ell_\beta & I \\ \ell_\alpha & J_\alpha & \lambda \end{Bmatrix} \left(S^I_{\alpha\beta} - \delta^I_{\alpha\beta}\right). \end{aligned} \tag{18}$$

3.2. Special cases of moments

Here we consider the moments for often used special cases of the coupled channel problem.

(a) *Only a single multipole operator Q_λ is active*: in this case we can resolve equation (15) directly for the moment $b^\lambda_{\alpha\beta}$ or we take equation (18). The S-matrix elements have a given dependence on the quantum number I of angular momentum in the first Born approximation, namely

$$\begin{aligned} S^I_{\alpha\beta} - \delta^I_{\alpha\beta} = -\frac{4\mathrm{i}\mu k_\alpha}{\hbar^2} \mathrm{i}^{\ell_\beta - \ell_\alpha} (-1)^{J_\alpha + \lambda} \frac{1}{\sqrt{4\pi}} \sqrt{(2\ell_\alpha+1)(2\lambda+1)(2\ell_\beta+1)} \\ \times \begin{pmatrix} \ell_\alpha & \lambda & \ell_\beta \\ 0 & 0 & 0 \end{pmatrix} b^\lambda_{\alpha\beta} (-1)^I \begin{Bmatrix} \ell_\alpha & \lambda & \ell_\beta \\ J_\beta & I & J_\alpha \end{Bmatrix}. \end{aligned} \tag{19}$$

The exact S-matrix slightly deviates from this form in its dependence on the quantum number I and, therefore, equation (18) which contains the sum over I yields averaged values of $b^{\lambda}_{\alpha\beta}$, whereas the direct solution of equation (15) leads to moments $b^{\lambda}_{\alpha\beta}$ depending weakly on I.

(b) *The elastic channel β has the intrinsic ground state with $J_\beta = 0$:* if $J_\beta = 0$, then $I = \ell_\beta$, $J_\alpha = \lambda$ and we obtain with equation (18):

$$b^{\lambda}_{\alpha\beta} = \frac{\mathrm{i}\hbar^2\sqrt{4\pi}}{4\mu k_\alpha}\mathrm{i}^{\ell_\alpha+\ell_\beta}\left(\sqrt{2\ell_\alpha+1}\begin{pmatrix}\ell_\alpha & \lambda & \ell_\beta\\ 0 & 0 & 0\end{pmatrix}\right)^{-1} \times \left(S^{I=\ell_\beta}_{\alpha\beta} - \delta^{I=\ell_\beta}_{\alpha\beta}\right)\Delta(J_\alpha\ell_\alpha I=\ell_\beta)\Delta(\ell_\alpha\ell_\beta\lambda). \tag{20}$$

3.3. Coupling matrix with the method of Backus and Gilbert

Equation (18) represents the moments of the diagonal and transition potentials. The coefficients $b^{\lambda}_{\alpha\beta}$ are known from the knowledge of the given S-matrix. As in the one-channel case [14], equation (18) can be resolved for $\langle i\|Q_\lambda\|j\rangle$ with $i = (\nu_i, J_i)$, $i = 1, \ldots, K$, by the method of Backus and Gilbert [17, 18]. We introduce the following ansatz for the coupling matrix $\left(b^{\lambda}_{\alpha\beta} = b^{\lambda}_{i\ell_\alpha, j\ell_\beta}\right)$:

$$\langle i\|Q_\lambda(r,\xi)\|j\rangle_{I_{\max}} = \sum_{\{\ell_\alpha,\ell_\beta\}=0}^{I_{\max}} h^{\lambda}_{i\ell_\alpha,j\ell_\beta}(r)b^{\lambda}_{i\ell_\alpha,j\ell_\beta} = \sum_{\{\ell_\alpha,\ell_\beta\}=0}^{I_{\max}} h^{\lambda}_{i\ell_\alpha,j\ell_\beta}(r)\int_0^a r'^2\,\mathrm{d}r' j_{\ell_\alpha}(k_ir')j_{\ell_\beta}(k_jr')\langle i\|Q_\lambda(r',\xi)\|j\rangle. \tag{21}$$

The notation $\{\ell_\alpha, \ell_\beta\}$ means that the sum runs over pairs of ℓ_α and ℓ_β which are allowed according to equation (18) where the sum over I is restricted to a maximum value $I_{\max}$. We introduced the functions $h^{\lambda}_{i\ell_\alpha,j\ell_\beta}(r)$ as expansion coefficients which have to be determined. In order that equation (21) holds, it follows that:

$$A^{\lambda,I_{\max}}_{i,j}(r,r') = \sum_{\{\ell_\alpha,\ell_\beta\}=0}^{I_{\max}} h^{\lambda}_{i\ell_\alpha,j\ell_\beta}(r)\,j_{\ell_\alpha}(k_ir')\,j_{\ell_\beta}(k_jr')r'^2 \to \delta(r-r'). \tag{22}$$

The sum on the left-hand side approaches the δ-function only for $I_{\max}\to\infty$ as explained in [14]. For finite values of $I_{\max}$ we can only reach an approximate expression. This can be achieved by requiring

$$\int_0^a A^{\lambda,I_{\max}}_{i,j}(r,r')\,\mathrm{d}r' = \sum_{\{\ell_\alpha,\ell_\beta\}=0}^{I_{\max}} h^{\lambda}_{i\ell_\alpha,j\ell_\beta}(r)F_{i\ell_\alpha,j\ell_\beta} = 1 \tag{23}$$

with

$$F_{i\ell_\alpha,j\ell_\beta} = \int_0^a j_{\ell_\alpha}(k_ir')\,j_{\ell_\beta}(k_jr')r'^2\,\mathrm{d}r' \tag{24}$$

and

$$\int_0^a \left|A^{\lambda,I_{\max}}_{i,j}(r,r')\right|^2|r-r'|^\tau\,\mathrm{d}r' = \sum_{\substack{\{\ell_\alpha,\ell_\beta\}=0,\\ \{\ell_\gamma,\ell_\delta\}=0}}^{I_{\max}} h^{\lambda}_{i\ell_\alpha,j\ell_\beta}(r)h^{\lambda *}_{i\ell_\gamma,j\ell_\delta}(r)F_{i\ell_\alpha,j\ell_\beta;i\ell_\gamma,j\ell_\delta}(r) = \min \tag{25}$$

with

$$F_{i\ell_\alpha,j\ell_\beta;i\ell_\gamma,j\ell_\delta}(r) = \int_0^a j_{\ell_\alpha}(k_ir')\,j_{\ell_\beta}(k_jr')\,j_{\ell_\gamma}(k_ir')\,j_{\ell_\delta}(k_jr')r'^4|r-r'|^\tau\,\mathrm{d}r'. \tag{26}$$

Condition (25) is the optimality condition for the δ-sequence $A_{i,j}^{\lambda,I_{\max}}(r,r')$, which is concentrated near $r = r'$. We take $\tau = 2$ here as it was set by Backus and Gilbert [17, 18]. An error estimate of the Backus–Gilbert method is considered in [20]. In our case the error depends on the maximum angular momentum $I_{\max}$, but needs a complex mathematical study to be given explicitly. We follow here a more practical standpoint by comparing the errors in the test examples with exact given coupling potentials as discussed in section 4.

The system of equations (23) and (25) has a unique solution for the expansion coefficients. Since the integrals (24) and (26) are real functions, it follows from the minimalization of (25) with the normalization condition (23) that the functions $h^{\lambda}_{i\ell_\alpha,j\ell_\beta}(r)$ are real. For conciseness let us introduce the notation $\nu = (i\ell_\alpha, j\ell_\beta) = 1, 2, \ldots, \nu_{\max}$, where the index ν counts the different possible combinations, allowed by angular momentum algebra for a coupling potential of multipolarity λ and internal states i and j up to a maximal value $I_{\max}$ of total angular momentum I. Then the following minimalization procedure with respect to the unknown functions $h^{\lambda}_{\nu}(r)$ is carried out by using a Lagrange multiplier $\eta^{\lambda}(r)$ depending on r and λ:

$$0 = \delta \int_0^a \left(\left| A_{i,j}^{\lambda,I_{\max}}(r,r') \right|^2 |r - r'|^2 + \eta^{\lambda}(r) A_{i,j}^{\lambda,I_{\max}}(r,r') \right) \mathrm{d}r'$$
$$= \sum_{\{\ell_\alpha,\ell_\beta\}=0}^{I_{\max}} \left(\sum_{\{\ell_\alpha',\ell_\beta'\}=0}^{I_{\max}} 2F_{\nu\nu'}(r) h^{\lambda}_{\nu'}(r) + F_\nu \eta^{\lambda}(r) \right) \delta h^{\lambda}_{\nu}(r) = 0. \tag{27}$$

This leads to the following system of equations:

$$\sum_{\{\ell_\alpha',\ell_\beta'\}=0}^{I_{\max}} 2F_{\nu\nu'}(r) h^{\lambda}_{\nu'}(r) + F_\nu \eta^{\lambda}(r) = 0. \tag{28}$$

Further we have to fulfil equation (23)

$$\sum_{\{\ell_\alpha,\ell_\beta\}=0}^{I_{\max}} F_\nu h^{\lambda}_{\nu}(r) = 1. \tag{29}$$

Equations (28) and (29) constitute a system of linear inhomogeneous equations of dimensions $\nu_{\max} + 1$. This system has to be solved for the $\nu_{\max}$ unknown quantities $h^{\lambda}_{\nu}(r)$ and the Lagrange multiplier $\eta^{\lambda}(r)$ where r plays the role of a parameter (or index) only. The system has a unique solution for each value of r and λ under the condition that the determinant formed with the coefficients $2F_{\nu\nu'}(r)$ and F_ν does not vanish. It has to be solved for discrete values of r. Then the inverted coupling potentials are obtained with (21):

$$\langle i \| Q_\lambda(r,\xi) \| j \rangle_{I_{\max}} = \sum_{\{\ell_\alpha,\ell_\beta\}=0}^{I_{\max}} b^{\lambda}_{\nu} h^{\lambda}_{\nu}(r). \tag{30}$$

The quality of this result is ultimately related to the limits of the first Born approximation since we approximated the interaction matrix (14) with the free solution in (14).

4. Results

In the following calculations, we assume two internal states $i = 1$ and 2 and assume $k_1 = k_2 = k$ which means that both the intrinsic states have the same energy. Further we set $\hbar^2/\mu = 40$ MeV fm^2.

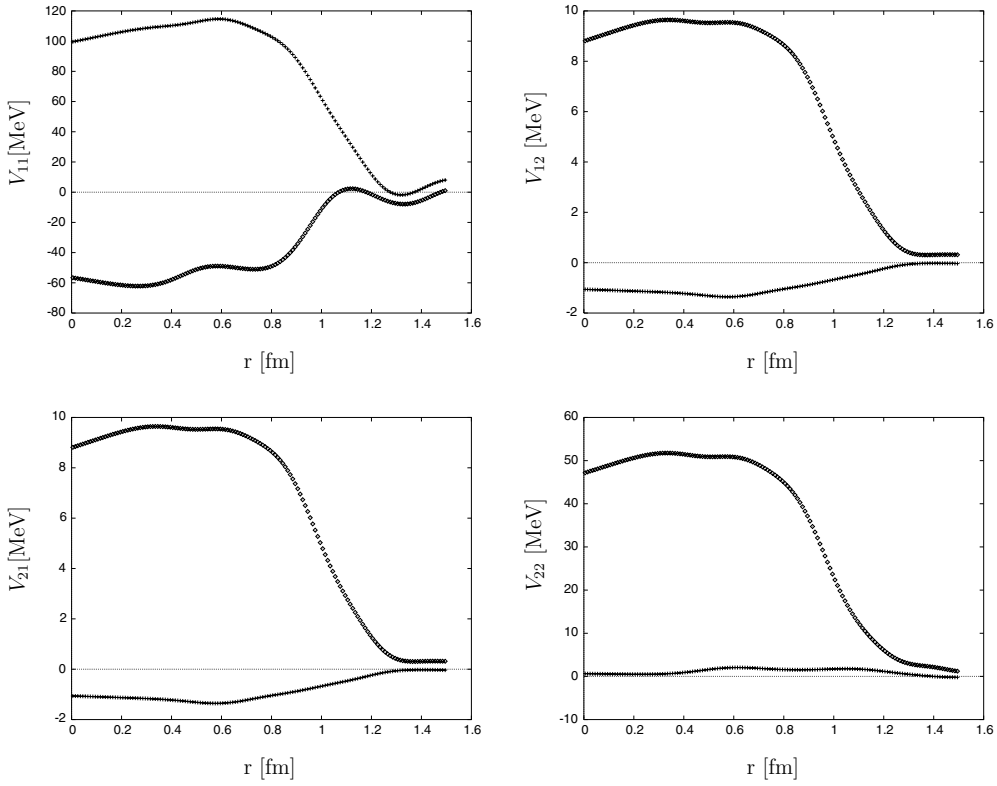

Figure 1. Inverted potential matrix calculated from the S-matrix obtained with $\hat{V}$ given in equation (33). The excitation energy is set to zero. The further parameters are $k = 5$ fm^{-1}, $\hbar^2/\mu = 40$ MeV fm^2, $a = 1.4$ fm and $I_{\max} = 8$.

4.1. Inversion for monopole-type coupling

As examples we first choose the case of the inversion of a S-matrix belonging to a coupling potential of monopole type between two intrinsic channels $i = 1$ and 2 which both have angular momenta $J_i = 0$. The coupling matrix in equation (6) can be written for $\lambda = 0$:

$$V_{ij}(r) = \langle i|\hat{W}(r,\xi)|j\rangle = \frac{1}{\sqrt{4\pi}}\langle i|Q_0(r,\xi)|j\rangle = \frac{\hbar^2}{2\mu}U^{I=\ell_\alpha}_{i\ell_\alpha,j\ell_\beta=\ell_\alpha}(r) \tag{31}$$

and

$$\begin{aligned} b^{\lambda=0}_{i\ell_\alpha,j\ell_\beta=\ell_\alpha} &= \int_0^a r'^2\,\mathrm{d}r'\, j_{\ell_\alpha}(k_i r')\, j_{\ell_\alpha}(k_j r')\sqrt{4\pi}\, V_{ij}(r') \\ &= \frac{\mathrm{i}\hbar^2\sqrt{4\pi}}{4\mu k_i}\left(S^{I=\ell_\alpha}_{i\ell_\alpha,j\ell_\alpha} - \delta^{I=\ell_\alpha}_{\alpha,\beta}\right). \end{aligned} \tag{32}$$

(a) *Coupling matrix with box potentials*: box potentials are the most sensitive potentials for a test of the inversion method because of their unsteady behaviour at the surface. For the coupling matrix we set complex box potentials,

$$\hat{V} = \begin{pmatrix} 100 - \mathrm{i}50 & 10 - \mathrm{i} \\ 10 - \mathrm{i} & 50 \end{pmatrix} \text{MeV for } r < 1 \text{ fm} \tag{33}$$

and $\hat{V} = 0$ for $r > 1$ fm.

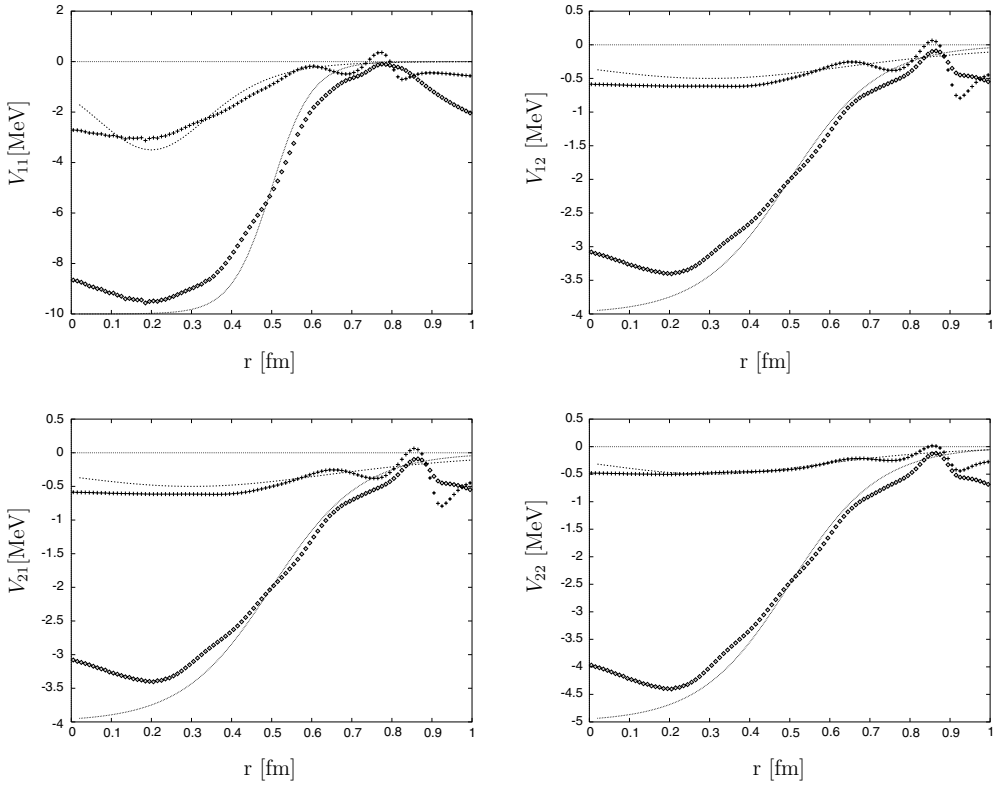

Figure 2. Inverted coupling matrix obtained from the S-matrix calculated with the complex Woods–Saxon coupling matrix with parameters given in table 1. The excitation energy is set to zero. The further parameters are $k = 5$ fm^{-1}, $\hbar^2/\mu = 40$ MeV fm^2, $a = 0.9$ fm and $I_{\max} = 6$. The exact coupling potentials are shown by thin curves and the inverted potentials by thick curves.

Table 1. Input parameters for the coupling matrix $\hat{V}$ defined in equation (33) and used in figures 2 and 3.

		V^0_{ij} (MeV)	R^r_{ij} (fm)	d^r_{ij} (fm^{-1})	W^0_{ij} (MeV)	R^i_{ij} (fm)	d^i_{ij} (fm^{-1})
	V_{11}	−10.0	0.5	10.0	−7.0	0.2	10.0
Figure 2	$V_{12} = V_{21}$	−4.0	0.5	7.5	−1.0	0.3	2.5
	V_{22}	−5.0	0.5	7.5	−1.0	0.3	5.0
	V_{11}	−1.0	1.5	2.0	−2.0	0.7	1.0
Figure 3	$V_{12} = V_{21}$	−0.6	1.5	3.5	−1.0	0.7	3.0
	V_{22}	−2.0	1.5	2.0	−0.5	1.0	2.0

We calculated the S-matrix analytically for $k = 5$ fm^{-1} and inverted it with the method described in section 3 by using $I_{\max} = 8$. The results of the inversion are shown in figure 1. The widths of the fall-off of the potentials around $r = 1$ fm indicate the quality of the method. The validity of the first Born approximation is determined by the inequalities $|v| \ll 1$ for $ka \ll 1$ and $|v|/(ka) \ll 1$ for $ka \gg 1$ with $v = \mu V a^2/\hbar^2$ and the range parameter a of the potential [21–23]. For $ka = 5$ and $V = -100$ MeV we find $|v|/(ka) = 0.5$, which means that the inversion method is at the limits of validity of the

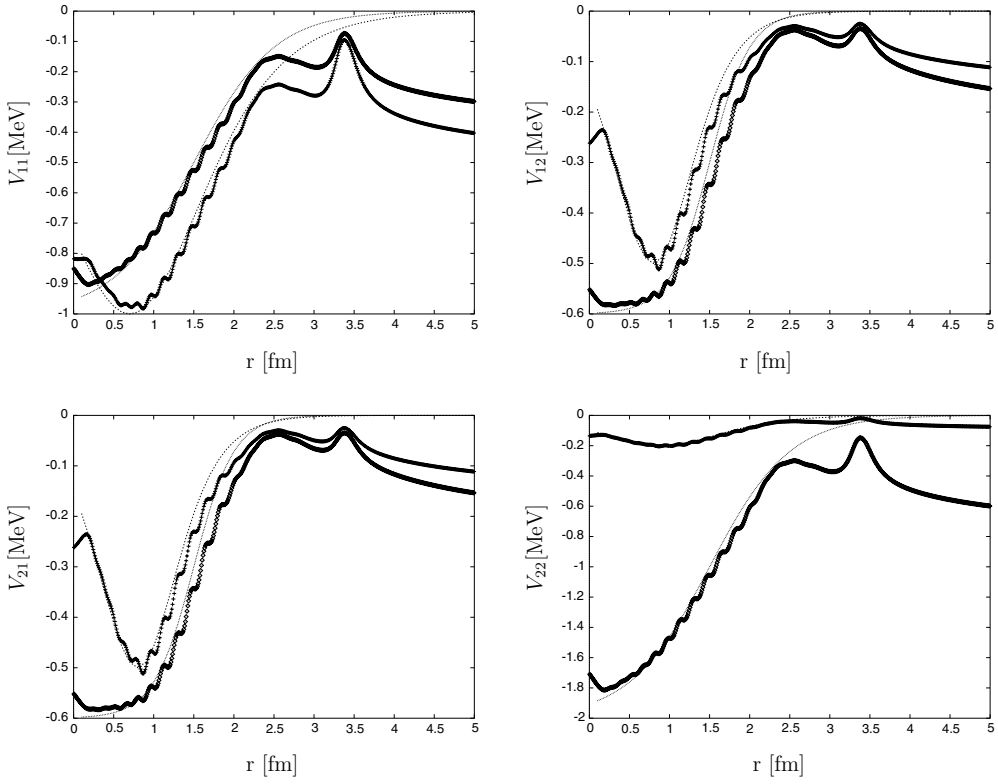

Figure 3. Inverted coupling matrix obtained from the S-matrix calculated with the complex Woods–Saxon coupling matrix with parameters given in table 1. The excitation energy is set to zero. The further parameters are $k = 1$ fm^{-1}, $\hbar^2/\mu = 40$ MeV fm^2, $a = 3.5$ fm and $I_{\max} = 6$. The exact coupling potentials are shown by thin curves and the inverted potentials by thick curves.

first Born approximation in the considered case. Therefore, it is surprising how well the assumed potential values are reached at smaller values of r.

(b) *Coupling matrix with Woods–Saxon potentials*: next we consider a coupling matrix with complex Woods–Saxon potentials, assuming

$$V_{ij}(r) = \frac{V_{ij}^0}{1 + \exp\left(d_{ij}^r\left(r - R_{ij}^r\right)\right)} + \mathrm{i}2\frac{W_{ij}^0 \exp\left(d_{ij}^i\left(r - R_{ij}^i\right)\right)}{\left(1 + \exp\left(d_{ij}^i\left(r - R_{ij}^i\right)\right)\right)^2}. \tag{34}$$

The values of the constants V_{ij}^0, W_{ij}^0, $R_{ij}^{r,i}$ and $d_{ij}^{r,i}$ used in the calculations are listed in table 1. As input values for the inversion procedure we calculated the S-matrix numerically with a precision of 10^{-5}. The results of the inversion are shown in figure 2, calculated with $k = 5$ fm^{-1}, $a = 0.9$ fm and $I_{\max} = 6$, and in figure 3, calculated with $k = 1$ fm^{-1}, $a = 3.5$ fm and $I_{\max} = 6$. The overall reproduction of the input potential for $r \leqslant a$ is fair. For $r > a$ the method starts to fail.

4.2. Inversion for dipole-type coupling

The next example we consider is a dipole-type coupling potential acting between an intrinsic ground state with $J_1 = 0$ and an excited intrinsic state with $J_2 = 1$. Using equation (20) with

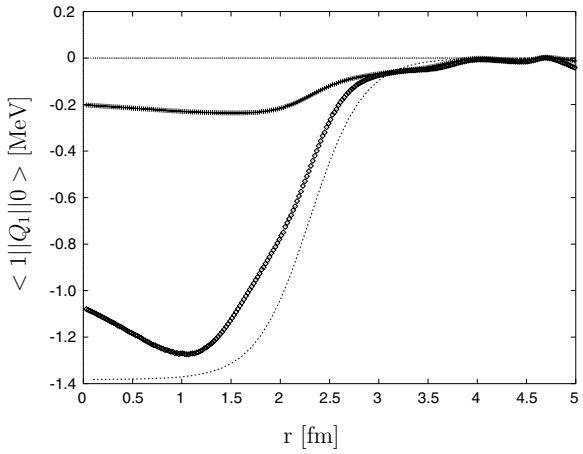

Figure 4. Real and imaginary parts (thick curves) of the dipole coupling $\langle J_2 = 1 \| Q_1 \| J_1 = 0 \rangle$ obtained by inversion of the S-matrix calculated with a real dipole coupling potential of Woods–Saxon form: $\langle J_2 = 1 \| Q_1 \| J_1 = 0 \rangle = -1.4$ MeV$/(1 + \exp(3.5(r/\text{fm} - 2.3)))$ (thin curve). The intrinsic ground state (no 1) has $J = 0$ and the excited state (no 2) $J = 1$. The excitation energy is set to zero. The further parameters are $k = 1$ fm^{-1}, $\hbar^2/\mu = 40$ MeV fm^2, $a = 4.25$ fm and $I_{\max} = 6$.

$\lambda = 1$, $J_\beta = J_1 = 0$, $I = \ell_\beta$, $J_\alpha = J_2 = 1$, $\ell_\alpha = \ell_\beta \pm 1$, we obtain

$$b^1_{2\ell_\alpha = \ell_\beta + 1, 1\ell_\beta} = \frac{\hbar^2\sqrt{4\pi}}{4\mu k_2}\sqrt{\frac{2\ell_\beta + 1}{\ell_\beta + 1}}\, S^{I=\ell_\beta}_{2\ell_\alpha = \ell_\beta + 1, 1\ell_\beta}, \tag{35}$$

$$b^1_{2\ell_\alpha = \ell_\beta - 1, 1\ell_\beta} = \frac{\hbar^2\sqrt{4\pi}}{4\mu k_2}\sqrt{\frac{2\ell_\beta + 1}{\ell_\beta}}\, S^{I=\ell_\beta}_{2\ell_\alpha = \ell_\beta - 1, 1\ell_\beta}. \tag{36}$$

With these relations one can now calculate the reduced matrix element $\langle J_2 = 1 \| Q_1 \| J_1 = 0 \rangle$ according to the inverse method explained in section 3.3. The reduced coupling matrix was chosen as a real Woods–Saxon potential with parameters $V^0_{12} = -V^0_{21} = 1.4$ MeV, $R^r_{12} = R^r_{21} = 2.3$ fm and $d^r_{12} = d^r_{21} = 3.5$ fm^{-1}. The parameters were set $k = 1$ fm^{-1}, $a = 4.25$ fm and $I_{\max} = 6$. The result of the inversion is shown in figure 4 for the obtained real and imaginary coupling potentials $\langle J_2 = 1 \| Q_1 \| J_1 = 0 \rangle$ in comparison with the exact real potential used in the calculation of the S-matrix.

5. Summary and conclusions

We introduced an approximative new method for inverting a quantum coupled channel problem with local coupling potentials at fixed energy. The method used is based on the procedure of Ramm, who considered the elastic inverse problem, and on the first Born approximation by replacing exact coupled wavefunctions by free solutions. The limits of the first Born approximation were investigated by Kohn [21] and reviewed in textbooks, e.g. by Schiff [22] and Messiah [23]. In the appendix, we give a derivation of the error of the potential as a function of the difference of the exact S-matrix elements and those of the first Born

Table 2. Estimates for the validity of the first Born approximation in the examples shown in the figures. The range a is that used in the calculations and $|V|$ is the maximal absolute value of the potential matrix. The conditions for the first Born approximation are $|v| \ll 1$ if $ka \ll 1$ and $|v|/ka \ll 1$ if $ka \gg 1$.

Figure no	a (fm)	ka	V (MeV)	$\|v\| = \mu a^2 \|V\|/\hbar^2$	$\|v\|/ka$
1	1.4	7	−100	4.9	0.7
2	0.9	4.5	−10	0.203	0.045
3	3.5	3.5	−2	0.613	0.175
4	4.25	4.25	−1.4	0.632	0.149

approximation. Setting $v = \mu V a^2/\hbar^2$ where a is the range of the potential, the first Born approximation is justified for $|v| \ll 1$ if $ka \ll 1$ and for $|v|/ka \ll 1$ if $ka \gg 1$. In table 2, we present estimates for v in relation to ka as used in the figures. In all cases we have $ka > 1$ and $|v|/ka < 1$. We calculated near the limit of the Born approximation in order to test the quality of the new procedure. At the moment, a definite error estimate for the coupling potentials cannot be given by us. It depends on the potential matrix, on the interaction radius a and the maximum angular momentum $I_{\max}$. To date, we can only derive a partial error estimate as given in the appendix.

Usually differential cross sections in and between all reaction channels may not be measured which has the consequence that the S-matrix cannot be completely deduced in praxis from the experimental cross sections and, therefore, is only partly known. However, in our procedure an incomplete S-matrix is sufficient to obtain the coupling potentials between the measured reaction channels since we apply as approximation a first-order perturbation theory with one-step transitions between the channels. An exact inversion theory has to take into account the effects of more-step couplings and needs the complete S-matrix as starting point. For example, the modified Newton–Sabatier method for coupled channels [12, 13] starts with the complete S-matrix. In this regard, we would like to mention the proposal to compare the modified Newton–Sabatier method and the inverse method based on the Born approximation. This has not yet been carried out.

Two extensions of this work await completion. Firstly, in most applications one comes across reactions between charged particles, e.g., in nuclear and atomic physics. In this case the Coulomb potential reaches up to infinity and is not restricted to a finite range $r < a$. This problem can be reduced by a transformation of the S-matrix to the case of uncharged particles interacting with a finite coupling as considered here. The method is quite similar to that already used for elastic scattering [24]. The extension of our method to charged particles is needed for realistic applications. All reactions where the use of the first Born approximation is justified could be studied within the method. As an interesting example, we mention the reaction $H^+ + H$ or He at energies $E_{lab} \geqslant 100$ keV considered in atomic physics [25]. We plan to apply our inverse method to this reaction.

Secondly, further progress in this work can be achieved with an iterative method. One first carries out the inverse method described in this paper and finds the coupling matrix and the corresponding wavefunctions in the first Born approximation. With these quantities one is able to formulate the inversion procedure in the second and higher Born approximations. Hence, the method described here can iteratively be repeated and should in principle lead from the complete S-matrix to the exact coupling matrix if the Born series converges. Such an iterative procedure which has not been yet undertaken should be first tested for the case of elastic scattering before it is transferred to the coupled case. Compared with the first Born approximation, the numerics will be more complex in the iteration calculations and first needs

to be tested. In an analogous manner, an inverse method based on the widely used distorted Born approximation can be developed and applied.

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Appendix. Estimation of the quality of inversion

The error estimate for the inversion problem requires precise scattering data. In [26], Ramm derived an error estimate for the three-dimensional scattering problem with noisy discrete fixed energy data. Let $A_\delta(\alpha', \alpha)$ be the noisy scattering amplitude and $A(\alpha', \alpha)$ the exact one with $\sup_{\alpha', \alpha \in S^2} |A_\delta(\alpha', \alpha) - A(\alpha', \alpha)| < \delta$, then Ramm gave an error estimate of the Fourier transform of the potential

$$\tilde{q}(\mathbf{k}) = \int_{R^2} \exp(-\mathrm{i}\mathbf{k}\mathbf{r}) q(\mathbf{r}) d^3 r : \tag{A.1}$$

$$\sup_{|\mathbf{k}| \leqslant k_0} |\tilde{q}(\mathbf{k}) - \tilde{q}_\delta(\mathbf{k})| \leqslant C(\ln|\ln\delta|)^2 / |\ln\delta|, \tag{A.2}$$

where $\tilde{q}_\delta(\mathbf{k})$ is obtained from $A_\delta(\alpha', \alpha)$ with an inversion procedure. This estimate shows that a very small value of δ is needed to minimize the right-hand side of (A.2). The right-hand side gets smaller with smaller values of δ for $\delta < \exp(-\exp(2)) = 0.000\,618$. However, it is experimentally nearly impossible to measure the scattering amplitude, respectively, the S-matrix elements with such a high precision. Therefore, we discuss here an estimate which regards the first Born approximation used in our approximate method.

According to equations (11), (13) and (14) we can write

$$S^I_{\alpha\beta} - S^{I,B1}_{\alpha\beta} = -2\mathrm{i} \int_0^a r'^2 \, \mathrm{d}r' k_\alpha j_{\ell_\alpha}(k_\alpha r') \sum_\gamma U^I_{\alpha\gamma}(r') \big(R^I_{\gamma\beta}(r') - \delta^I_{\gamma\beta} j_{\ell_\beta}(k_\beta r') \big), \tag{A.3}$$

where $S^{I,B1}_{\alpha\beta}$ is the S-matrix in the first Born approximation and given in equation (15). Inserting equation (8) into (A.3) we find

$$\begin{aligned} S^I_{\alpha\beta} - S^{I,B1}_{\alpha\beta} = -2 \int_0^a r'^2 \, \mathrm{d}r' k_\alpha j_{\ell_\alpha}(k_\alpha r') \sum_\gamma U^I_{\alpha\gamma}(r') \\ \times \int_0^a r''^2 \, \mathrm{d}r'' k_\gamma j_{\ell_\gamma}(k_\gamma r_<) h^{(1)}_{\ell_\gamma}(k_\gamma r_>) \sum_\delta U^I_{\gamma\delta}(r'') R^I_{\delta\beta}(r''). \end{aligned} \tag{A.4}$$

Up to here the procedure is exact. To proceed further and to end with some useful results, we simplify the considerations to the uncoupled case: $S^I_{\alpha\beta} \to S^\ell$ and $U^I_{\alpha\gamma}(r) \to (2\mu/\hbar^2) V(r)$, approximate $R^I_{\delta\beta}(r'') \to j_\ell(kr'')$ which means the second Born approximation for S^ℓ and replace $V(r)$ by a constant V in the interval $0 \leqslant r < a$ and zero otherwise. Then we obtain

$$S^\ell - S^{\ell,B1} = -2 \left(\frac{2\mu V}{k^2 \hbar^2} \right)^2 F(ka, \ell) \tag{A.5}$$

with

$$\begin{aligned} F(ka, \ell) = \left(\int_0^{ka} x^2 j^2_\ell(x) \, \mathrm{d}x \right)^2 + \mathrm{i} \int_0^{ka} x^2 j_\ell(x) \, \mathrm{d}x \\ \times \left(n_\ell(x) \int_0^x x'^2 \, \mathrm{d}x' j^2_\ell(x') + j_\ell(x) \int_x^{ka} x'^2 \, \mathrm{d}x' n_\ell(x') j_\ell(x') \right). \end{aligned} \tag{A.6}$$

For the special value $\ell = 0$ it yields

$$F(ka, \ell = 0) = \frac{1}{4}\,(ka - \sin(ka)\cos(ka))^2 + \mathrm{i}\left(-\frac{ka}{8} + \frac{1}{2}ka\cos^2(ka) - \frac{1}{8}\sin(ka)\cos(ka)(1 + 2\cos^2(ka))\right). \tag{A.7}$$

The absolute value of the last expression (A.7) can be approximated with a relative precision of a maximal factor of 2 by

$$|F(ka, \ell = 0)| \approx \frac{\frac{2}{15}(ka)^5}{1 + \frac{8}{15}(ka)^3}. \tag{A.8}$$

This formula has the correct behaviour for $ka \to 0$ and $ka \to \infty$. Using (A.8), we can estimate the range of applicability of the first Born approximation. For the two limiting cases, we find the known conditions for the first Born approximation:

$$ka < 1: \qquad \frac{\mu|V|a^2}{\hbar^2}\sqrt{ka} \ll 1, \tag{A.9}$$

$$ka > 1: \qquad \frac{\mu|V|a}{\hbar^2 k} \ll 1. \tag{A.10}$$

Assuming that the S-matrix in the first Born approximation is given, the potential strength of a box potential is exactly calculable by

$$V = \frac{1 - S^{\ell,B1}}{2\mathrm{i}\left(\frac{2\mu}{\hbar^2k^2}\right)\int_0^{ka} x^2 j_\ell^2(x)\,\mathrm{d}x}. \tag{A.11}$$

However, when we use the exact S-matrix for the determination of the potential strength by the same formula we get an error δV in V:

$$V + \delta V = \frac{1 - S^{\ell}}{2\mathrm{i}\left(\frac{2\mu}{\hbar^2k^2}\right)\int_0^{ka} x^2 j_\ell^2(x)\,\mathrm{d}x}. \tag{A.12}$$

This error can be estimated by applying (A.5):

$$\delta V = \frac{S^{\ell,B1} - S^{\ell}}{2\mathrm{i}\left(\frac{2\mu}{\hbar^2k^2}\right)\int_0^{ka} x^2 j_\ell^2(x)\,\mathrm{d}x} = \frac{-\mathrm{i}\left(\frac{2\mu}{\hbar^2k^2}\right)V^2F(ka, \ell)}{\int_0^{ka} x^2 j_\ell^2(x)\,\mathrm{d}x}. \tag{A.13}$$

Then setting $\ell = 0$ and inserting (A.7) and (A.8), we obtain an approximate estimate

$$\left|\frac{\delta V}{V}\right| \approx \frac{\frac{4}{5}\mu|V|a^2}{\hbar^2\left(1 + \frac{4}{5}ka\right)} \tag{A.14}$$

with the result $|\delta V/V| \approx \mu|V|a^2/\hbar^2$ for $ka < 1$ and $\approx \mu|V|a/(\hbar^2 k)$ for $ka > 1$. These estimates have the same form as those derived for the validity of the Born approximation. Estimates for the potentials shown in the figures are presented in table 2.

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