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Study of the Cox–Thompson inverse scattering method with a Coulomb potential

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Abstract
In order to learn more about the precision of the inversion by the Cox–Thompson method, we investigated the inversion of phase shifts of a singular potential, namely of a Coulomb potential. Using asymptotically Riccati–Bessel functions as reference functions, we could only approximately reproduce the singularity of the Coulomb potential at the origin. We also show uncertainties in the inverted potential due to different minima in the minimization solution of the nonlinear equations of the Cox–Thompson procedure. As a result, we conclude that one has to take much care with the inversion of experimental phase shifts suffering from measurement errors.

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1. Introduction

In this short paper, we test the precision of the Cox–Thompson method [1, 2] by solving the inverse scattering problem at fixed energy for a Coulomb potential. The phase shifts of the Coulomb problem are analytically known [3]. Further, the Coulomb potential is far reaching and has a singularity of first order at the origin. Since the Cox–Thompson method published so far for practical applications in the literature [2, 4] works for potentials with a finite range, we first transform the Coulomb phases to the phases of a new potential which is given as

$$\begin{aligned} &V(r) = V_C(r) - V_C(r = R) \qquad \text{for} \qquad r \leqslant R, \\ &V(r) = 0 \qquad \text{for} \qquad r \geqslant R \end{aligned} \tag{1}$$

with the Coulomb potential

$$V_C(r) = \frac{1}{4\pi\varepsilon_0}\frac{q_1 q_2}{r}. \tag{2}$$

Here, r is the relative coordinate between the scattered particles with charges q_1 and q_2 and R is an arbitrary radius. The transformation of the pure Coulomb phases to the modified phases

δ_ℓ of the potential $V(r)$ in (1) is obtained by setting the logarithmic derivative of the Coulomb wavefunction equal to the logarithmic derivative of the wavefunction belonging to $V(r)$ at $r = R$ (see [6]):

$$\frac{\mathrm{d}}{\mathrm{d}r} \ln\left(\cos(\delta_\ell)\, j_\ell(kr) - \sin(\delta_\ell) n_\ell(kr)\right)|_{r=R} = \frac{\mathrm{d}}{\mathrm{d}r} \ln\left(F_\ell(k_C r)/(k_C r)\right)|_{r=R}. \tag{3}$$

The wavefunction $F_\ell(kr)$ is the regular Coulomb wavefunction and solves the differential equation [3]:

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}(kr)^2} + \left(1 - \frac{2\eta}{kr} - \frac{\ell(\ell+1)}{(kr)^2}\right)\right) F_\ell(kr) = 0, \tag{4}$$

where $\eta = \mu q_1 q_2/(4\pi\varepsilon_0\hbar^2 k)$ is the Sommerfeld parameter. The functions $j_\ell(kr)$ and $n_\ell(kr)$ are regular and irregular spherical Bessel functions, respectively, both solving the differential equation [3]:

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}(kr)^2} + \left(1 - \frac{\ell(\ell+1)}{(kr)^2}\right)\right) kr \begin{Bmatrix} j_\ell(kr) \\ n_\ell(kr) \end{Bmatrix} = 0. \tag{5}$$

The wave numbers k_C and k are related to the c.m. energy of the Coulomb problem:

$$E_{\text{c.m.}} = \frac{1}{2\mu} k_C^2 \hbar^2 \qquad \text{and} \qquad E_{\text{c.m.}} - V_C(r = R) = \frac{1}{2\mu} k^2 \hbar^2. \tag{6}$$

Solving (3) for δ_ℓ we find the formula which allows us to calculate the phases of the potential (1):

$$\delta_\ell = \arctan \frac{\frac{\mathrm{d}}{\mathrm{d}(kR)} j_\ell(kR) - C j_\ell(kR)}{\frac{\mathrm{d}}{\mathrm{d}(kR)} n_\ell(kR) - C n_\ell(kR)} \tag{7}$$

with

$$C = \frac{k_C}{k} \frac{\frac{\mathrm{d}}{\mathrm{d}(k_C R)}\left(F_\ell(k_C R)/(k_C R)\right)}{\left(F_\ell(k_C R)/(k_C R)\right)}. \tag{8}$$

These phase shifts correspond to the Schrödinger equation for $r \leqslant R$:

$$\left(-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\mathrm{d}^2}{\mathrm{d}r^2} r + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} + V_C(r)\right) \psi_\ell(r) = E_{\text{c.m.}} \psi_\ell(r). \tag{9}$$

This paper will make some statements about the precision of the Cox–Thompson method. We have chosen the potential $V(r)$ given by (1). The phase shifts are analytically known by (7). In the following we set the parameters in the Schrödinger equation (9) $\hbar^2/\mu = 1$ MeV fm^2, $q_1 = Z_1 e = 2e$ and $q_2 = Z_2 e = 2e$ and $R = 1$ fm in all calculations [7]. Z_1 and Z_2 are the charge numbers which have the values $Z_1 = Z_2 = 2$. We varied $E_{\text{c.m.}}$ in the range between 6 MeV and 100 MeV and took different maximal angular momenta denoted by $\ell_{\max}$. In table 1 we list the phase shifts up to $\ell_{\max} = 18$ for $E_{\text{c.m.}} = 10, 20, 50$ and 100 MeV obtained from (7).

Despite the fact that the theoretical formulation of the Cox–Thompson method dates back to as early as 1970, the difficult problem of constructing equations to be solved by using a finite set of phase shifts was first attacked in 2002/2003 by Apagyi *et al* [2]. The resulting equations are highly nonlinear and can presently only be solved by minimizing procedures. In contrast, this is not the case with the Newton–Sabatier method [8, 9] where one derives solvable linear equations. However, the large difference between both methods is that the Cox–Thompson method can express potentials with a first moment $\int_0^\infty r V(r)\,\mathrm{d}r \neq 0$ differently from zero, whereas the Newton–Sabatier method always yields potentials with a zero first moment. Here,

Table 1. The phase shifts of the potential (1) as a function of the quantum number ℓ of the angular momentum for $E_{\text{c.m.}} = 10$, 20, 50 and 100 MeV.

ℓ	δ_ℓ (10 MeV)	δ_ℓ (20 MeV)	δ_ℓ (50 MeV)	δ_ℓ (100 MeV)
0	−1.235 928 51	−1.563 266 77	−1.379 677 55	−1.152 577 04
1	−0.423 372 652	−0.845 253 161	−0.862 218 109	−0.765 991 439
2	−0.094 456 5003	−0.436 566 43	−0.589 636 714	−0.567 659 785
3	−0.012 146 3809	−0.183 622 48	−0.406 512 147	−0.436 368 785
4	−0.000 957 791 295	−0.056 347 1675	−0.279 610 676	−0.338 291 985
5	$-5.167\,916\,21 \times 10^{-5}$	−0.012 066 6237	−0.184 420 097	−0.263 765 573
6	$-2.050\,535\,54 \times 10^{-6}$	−0.001 841 950 66	−0.105 682 983	−0.202 424 452
7		−0.000 210 053 096	−0.048 778 9196	−0.151 401 622
8		$-1.864\,5179 \times 10^{-5}$	−0.017 570 7033	−0.111 478 243
9		$-1.328\,054\,58 \times 10^{-6}$	−0.004 936 486 93	−0.077 731 3484
10			−0.001 100 5313	−0.047 677 4367
11			−0.000 199 158 872	−0.024 457 5159
12			$-2.987\,629\,23 \times 10^{-5}$	−0.010 302 5557
13			$-3.780\,857\,67 \times 10^{-6}$	−0.003 568 679 41
14				−0.001 027 826 11
15				−0.000 249 706 347
16				$-5.189\,993\,49 \times 10^{-5}$
17				$-9.344\,584\,52 \times 10^{-6}$
18				$-1.473\,309\,79 \times 10^{-6}$

we do not want to discuss the possibility that these methods may not give an unique inverted potential (see e.g. [10]).

In section 2 we shortly sketch the Cox–Thompson method for the case that the potential vanishes for $r \geqslant R$ and in section 3 we present and discuss results of the inversion.

2. Equations of the Cox–Thompson method

In this section, we use dimensionless coordinates, potentials and operators:

$$\rho = kr, \qquad U(\rho) = V(r)/E, \qquad \hat{D}^U(\rho) = \rho^2 \left(\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} + 1 - U(\rho) \right), \tag{10}$$

where $E = k^2\hbar^2/(2\mu)$ is the energy.

First, we represent the scattering wavefunction $\phi_\ell^U(\rho)$ of the unknown potential $U(\rho)$ with a finite range in dependence of known wavefunctions of a given finite range reference potential $U_0(\rho)$ by using the Povzner–Levitan representation [11]:

$$\phi_\ell^U(\rho) = \phi_\ell^{U_0}(\rho) - \int_0^\rho \frac{\mathrm{d}\rho'}{\rho'^2} L_{U_0}^U(\rho, \rho') \phi_\ell^{U_0}(\rho'). \tag{11}$$

The wavefunctions fulfil the Schrödinger equations

$$\hat{D}^U(\rho)\phi_\ell^U(\rho) = \ell(\ell+1)\phi_\ell^U(\rho), \tag{12}$$

$$\hat{D}^{U_0}(\rho)\phi_\ell^{U_0}(\rho) = \ell(\ell+1)\phi_\ell^{U_0}(\rho). \tag{13}$$

In $\hat{D}^{U_0}$ the potential U is replaced by U_0. The function $\phi_\ell^U(\rho)$ in the form (11) fulfils the Schrödinger equation (12) if the kernel $L_{U_0}^U(\rho, \rho')$ solves the differential equation and the conditions:

$$\hat{D}^U(\rho)L_{U_0}^U(\rho, \rho') = \hat{D}^{U_0}(\rho')L_{U_0}^U(\rho, \rho') \qquad \text{and} \qquad L_{U_0}^U(\rho, 0) = L_{U_0}^U(0, \rho') = 0 \tag{14}$$

with the potential

$$U(\rho) = U_0(\rho) - \frac{2}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\left(\frac{L_{U_0}^U(\rho, \rho)}{\rho}\right). \tag{15}$$

In order to get the potential one has to find the kernel $L_{U_0}^U$ from a set of given phase shifts δ_ℓ with $\ell \in S$ at a fixed energy. Here, S denotes the set of all physical angular momentum quantum numbers ℓ of which the phase shifts are given and which are taken into account in the calculation. S is also the number of the used phase shifts. Cox and Thompson made the ansatz for finite range potentials U and U_0:

$$L_{U_0}^U(\rho, \rho') = \sum_{L\in T} A_L(\rho)u_L(\rho') \tag{16}$$

with the regular Riccati–Bessel functions [3] $u_L(\rho) = \rho \cdot j_L(\rho)$ and the new set of real numbers $L \in T$ where the numbers L are noninteger numbers in contrast to the integer ℓ values. With T we denote the set of nonphysical angular momenta L. Also T is a number counting the nonphysical angular momenta. The numbers S and T are equal: $S = T$. So the intersection of the sets S and T is empty; hence, we can write $S \cap T = \{\}$. In the following we simply set $U_0(\rho) = 0$. The $A_L(\rho)$ are determined by the linear equations

$$\sum_{L\in T} A_L(\rho)\frac{W[u_L(\rho), v_\ell(\rho)]}{\ell(\ell+1) - L(L+1)} = v_\ell(\rho), \qquad \ell \in S, \tag{17}$$

where the functions $v_\ell(\rho) = \rho \cdot n_\ell(\rho)$ are irregular Riccati–Bessel functions [3] and W is the Wronski determinant $W[a, b] = ab' - ba'$. The values of the numbers $L \in T$ are determined by minimizing the real quantity $f_{\min}$ obtained from the highly nonlinear equations [2, 4, 5, 7]:

$$\exp(2\imath\delta_\ell) - \frac{1 + \imath\mathcal{K}_\ell^+}{1 - \imath\mathcal{K}_\ell^-} = \epsilon_\ell \qquad \text{and} \qquad f_{\min} = \frac{1}{2}\sum_{\ell\in S}|\epsilon_\ell|^2. \tag{18}$$

The quantity $\mathcal{K}_\ell^\pm$ is given by

$$\mathcal{K}_\ell^\pm = \sum_{L\in T, \ell'\in S} [M_{\sin}]_{\ell L}\left[M_{\cos}^{-1}\right]_{L\ell'} \exp(\pm\imath(\ell - \ell')\pi/2), \qquad \ell \in S, \tag{19}$$

with

$$\begin{Bmatrix} M_{\sin} \\ M_{\cos} \end{Bmatrix} = \frac{1}{L(L+1) - \ell(\ell+1)} \begin{Bmatrix} \sin\left((\ell - L)\frac{\pi}{2}\right) \\ \cos\left((\ell - L)\frac{\pi}{2}\right) \end{Bmatrix}, \qquad \ell \in S, \qquad L \in T, \qquad S \cap T = \{\}. \tag{20}$$

3. Results

Since the modified Newton–Sabatier [12] and Cox–Thompson [1] methods expand the potential in the form of Bessel functions (see (15) and (16)), it is not clear from the first whether a potential with a singularity at $r = 0$ like $V(r)$ given in (1) can be represented. Therefore, we calculated the Cox–Thompson method with the phase shifts of $V(r)$ (see table 1) for different energies $E_{\text{c.m.}}$ and different numbers of phase shifts at fixed energies. We

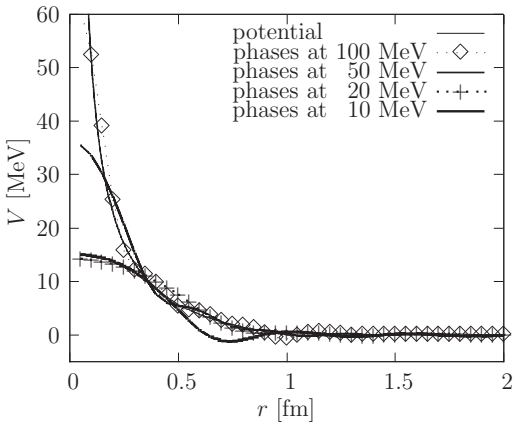

Figure 1. The potential $V(r)$ inverted with the phase shifts given in table 1 for different energies E_{cm}.

used double precision in a Fortran program [13] and minimized $f_{\min}$ to numbers of the order of about 10^{-21} with the Newton–Raphson and simulated annealing methods [14].

Figure 1 shows the result of the inversion of the phases given in table 1 for different energies $E_{\mathrm{c.m.}}$. These energies correspond to the Coulomb potential. The energies corresponding to the potential $V(r)$ (see (1)) are obtained by $E = E_{\mathrm{c.m.}} - V_C(r = R) = E_{\mathrm{c.m.}} - 5.76$ MeV. One can recognize that the singularity at $r = 0$ gets better simulated if the energy $E_{\mathrm{c.m.}}$ increases and more phase shifts up to 10^{-6} in precision with growing energy can contribute. The exact result with $V(r \geqslant R = 1\ \mathrm{fm}) = 0$ is approximately reproduced.

The classical turning point in the Coulomb potential at $r = R_t$ is calculated for $\ell = 0$ by $q_1 q_2/(4\pi\varepsilon_0 R_t) = E_{\mathrm{c.m.}}$. It results in $R_t = 0.576, 0.288, 0.115$ and 0.0576 fm for $E_{\mathrm{c.m.}} = 10, 20, 50$ and 100 MeV, respectively. Since classically and essentially quantum mechanically the charged particles do not approach each other closer than R_t, the phase shifts carry only little information about the potential for relative distances smaller than R_t. Therefore, we expect and can recognize in figure 1 that the quality of the inverted potentials gets smaller for $r < R_t$ (we let out the drawing of the values of R_t in figure 1 in order to have a clearer impression).

In figure 2 we present inverted potentials obtained with different numbers of the lowest phase shifts of the potential (1) at the fixed energy of $E_{\mathrm{c.m.}} = 100$ MeV. Together with the curve of figure 1 we choose the numbers as 9, 16 (figure 2) and 19 (figure 1). Whereas the curves for 9 and 19 phases can represent the potential satisfactorily, the curve with 16 phases deviates more from the given potential. This effect is visible from the values of L collected for the three cases shown in table 2. The L values for 9 and 19 phase shifts obtained from the minimization procedure of the nonlinear system of equations (see (18)) are very similar in contrast to those belonging to the case with 16 phase shifts. This can also be seen from the values of $f_{\min} = 1.34 \times 10^{-22}$, 1.59×10^{-21} and 1.35×10^{-22} which we reached for the cases with 9, 16 and 19 phase shifts, respectively. This difference in the solution minimum may be related to the singularities in the functions $A_{L\in T}(\rho)$ (see equation (17)) because, as a recent investigation shows [15] for the one phase shift case, such singularities are in an intimate connection with the non-unique solution of the Cox–Thompson method. Indeed, we numerically calculated the determinant of the matrix appearing in (17) and found a root at $\rho = 0.53$ with 16 L values and no roots with 9 and 19 L values. Without the help of a

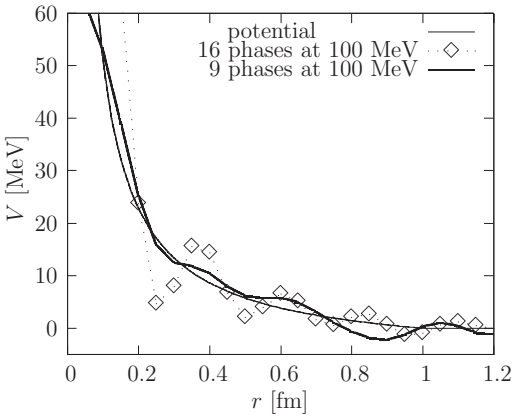

Figure 2. The potential $V(r)$ inverted with 9 and 16 phase shifts at the fixed energy $E_{\text{c.m.}} = 100$ MeV.

Table 2. The L values of the potential (1) as a function of the quantum number ℓ of the angular momentum for $E_{\text{c.m.}} = 100$ MeV calculated with the first 9, 16 and 19 phase shifts given in table 1 for $E_{\text{c.m.}} = 100$ MeV.

ℓ	L with 9 phases	L with 16 phases	L with 19 phases
0	0.393 977 723	−2.046 277 13	0.390 581 397
1	1.334 892 61	1.422 902 84	1.336 595 77
2	2.331 614 21	2.404 591 68	2.329 085 97
3	3.280 292 43	3.315 377 48	3.281 363 15
4	4.261 931 88	4.314 300 84	4.259 151 64
5	5.212 317 46	5.238 052 91	5.212 778 64
6	6.189 881 88	6.228 709 08	6.186 009 61
7	7.142 9849	7.161 821 91	7.142 580 07
8	8.128 340 87	8.150 400 83	8.118 4294
9		9.097 925 74	9.084 200 67
10		10.088 4535	10.064 9022
11		11.016 3934	11.007 5453
12		12.042 5884	12.027 0917
13		13.023 4869	13.017 4142
14		14.026 5585	14.015 2169
15		15.015 286	15.010 6764
16			16.010 8325
17			17.008 2256
18			18.008 4178

more sophisticated consideration one cannot know the correct minimum $f_{\min}$ in the case of experimental phase shifts. Therefore, it is difficult to recognize the true potential.

4. Conclusions

The study shows clearly that the Cox–Thompson method with Riccati–Bessel functions for the reference functions produces the Coulomb singularity with an increasing number of phase

shifts only in approximation. It is clear that the Cox–Thompson method with Coulomb wavefunctions as reference functions treats this problem with much higher precision [5]. However, in general one does not know in advance whether the given experimental phase shifts are related to a potential with or without a hardcore potential (singularity), and one would usually start with the Cox–Thompson method with the Riccati–Bessel reference functions. Therefore, the resulting inverted potential obtained with a finite number of experimental phase shifts of not too high a precision must be interpreted with much carefulness.

Our calculations at a single fixed energy with different numbers of phase shifts by minimizing (18) can lead to slightly different inverted potentials depending on which minimum the minimization procedures can reach. Because this ambiguity is difficult to control with the precision of the minimization, further theoretical improvements are necessary concerning the underlying uniqueness problem of the Cox–Thompson method.

From these investigations one has to conclude that more complex potentials like the Coulomb potential can probably not be calculated from a set of experimental phase shifts if a sufficient precision is prescribed. Small changes in the phase shifts and their number used in the inversion procedure are very sensitive to the reproduction of the correct shape of the true potential. These uncertainties in the inverted potential are of practical nature, but they are not caused by a mathematical incompleteness of the Cox–Thompson inversion procedure. Much care has to be taken with the inversion of experimental phase shifts which also suffer from measurement errors.

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