Determination of two-channel scattering amplitudes using unitarity

A. Purwanto, D. R. Lun, R. P. McEachran, and S. J. Buckman
Atomic and Molecular Physics Laboratories, Research School of Physical Sciences and Engineering, Australian National University, Canberra, ACT 0200, Australia
(Received 3 May 2000; published 9 January 2001)

A phase-shift analysis technique for two-channel scattering has been studied. The inputs to the study were the experimental differential cross sections and the unitarity condition was then used to extract the phase of the scattering amplitudes. A Newton iterative method based upon Frechet derivatives gave convergent results. The method was tested by using both simulated data and theoretical calculations for electron-helium scattering.

DOI: 10.1103/PhysRevA.63.022703 PACS number(s): 34.10.+x, 34.80.-i

I. INTRODUCTION

The determination of scattering amplitudes from experimental data is the first step in obtaining the interaction potentials using inverse-scattering methods [1]. Usually, the experimental data are the differential cross sections, $d\sigma_{fi}/d\Omega$, where i and f indicate the initial and final states of a multichannel scattering process, respectively. Here $d\sigma_{fi}/d\Omega$ is related to the corresponding scattering amplitude $f_{fi}(\theta)$ by the relationship

$$f_{fi}(\theta)=\sqrt{\frac{d\sigma_{fi}(\theta)}{d\Omega}}\exp[i\phi_{fi}(\theta)]. \tag{1}$$

The phase function $\phi_{fi}(\theta)$ of a scattering amplitude is not generally measured so it needs to be determined by theoretical means. The process of extracting the phase function from differential cross-section data is referred to as phase-shift analysis and there are various such techniques. A common approach is to parametrize the scattering amplitudes or their equivalent—the phase shifts or the scattering matrix—and to use a nonlinear fitting procedure to find the scattering amplitudes that best fit the data. The advantage of this approach is its wide applicability and that it does not require complete sets of angular data (from 0° to 180°). The disadvantage is that it is model-dependent and the question of existence and uniqueness of the solution cannot be addressed. A less common approach is to use a more global means, namely the unitarity theorem. This theorem translates into coupled nonlinear integral equations for the phase functions. The advantage of this approach is that the search for solutions is based on physical constraints and is model-independent. The disadvantage is the difficulty in solving the unitarity equations. Newton [2], Martin [3], Gerber and Karplus [4], and Atkinson *et al.* [5] have studied the unitarity equations in great detail. Their main interest was in the existence and the uniqueness of solutions. By the use of fix-point theorems, they obtained various domains for the differential cross sections, within which a unique solution to the unitarity equations was shown to exist and could be constructed by a simple iterative procedure. However, most physical circumstances lie outside these domains. In order to make use of the unitarity condition in phase-shift analysis, Lun *et al.* [6] recently used a Newton iterative method to solve the single unitarity equation for one-channel scattering. Although the Newton method cannot prove the uniqueness of the solution, it works even when the fix-point theorem method fails. This Newton method was applied to analyze data for neutron-α particle scattering at low energies and electron-water scattering at 1000 eV. Later Huber *et al.* [7] extended the method to scattering with spin-orbit interactions and tested the method with an optical model calculation for 1 MeV neutron-α particle scattering.

In view of these successes, the next step is to treat multichannel scattering cases. In order to obtain the complete scattering amplitude matrix for multichannel scattering, data for all energy-accessible scattering processes (open channels) are needed. Many experimental measurements have been made for multichannel scattering, but it is rare that a complete set of data is available because of the difficulty in obtaining data when the excited states are the initial scattering state. Recently, with the advancement of experimental technology, attempts are being considered to obtain such a complete data set for electron-helium scattering at energies above the first excitation threshold. This motivates, in part, our development of a phase-shift analysis technique for multichannel scattering. In this paper, we begin by studying unitarity for the simplest multichannel scattering process, namely the two-channel scattering of two spinless particles. Furthermore, the phase-shift analysis method developed here is also valid for electron-helium scattering at energies between the first and the second excitation thresholds when the differential cross section is spin-resolved. The extension to more than two channels is straightforward in principle, but involves a considerable increase in computational complexity.

II. THEORY

The generalized unitarity theorem, valid for any scattering process, is given by

$$\frac{4\pi}{|\mathbf{K}_i|}\,\mathrm{Im}\,f_{fi}(\mathbf{K}_f,\mathbf{K}_i)=\sum_m\int d\Omega_{K_m}f^*_{mf}(\mathbf{K}_m,\mathbf{K}_f)f_{mi}(\mathbf{K}_m,\mathbf{K}_i), \tag{2}$$

where Im denotes the imaginary part, the **K**'s are the momenta of the initial (i) and final (f) states, and the sum is over all open channels. We now consider the specific case of two-channel scattering where (a,b) and (c,d) are pairwise nonidentical, spinless particles giving rise to the following processes:

$$a+b\rightarrow a+b, \tag{3}$$

$$a+b\rightarrow c+d, \tag{4}$$

$$c+d\rightarrow c+d, \tag{5}$$

$$c+d\rightarrow a+b. \tag{6}$$

If time-reversal invariance holds, then the second and fourth of these processes are equivalent and we can omit the latter. We next define the dimensionless quantity as

$$A_k(x)=|\mathbf{K}_i|^{-1}\sqrt{\frac{d\sigma_{fi}}{d\Omega}\cos\theta},\quad x=\cos\theta, \tag{7}$$

where the subscript $k=1,2,3$ refers to the three processes in Eqs. (3)–(5). After some transformations, the unitarity equations [Eq. (2)] can be written as the following three equations for the phase functions φ_k:

$$A_1(x)\sin\varphi_1(x)=\int\int H(1,1)\cos[\varphi_1(y)-\varphi_1(z)]dy\,dz + \int\int H(2,2)\cos[\varphi_2(y)-\varphi_2(z)]dy\,dz, \tag{8}$$

$$A_2(x)\sin\varphi_2(x)=\int\int H(2,1)\cos[\varphi_2(y)-\varphi_1(z)]dy\,dz + \int\int H(2,3)\cos[\varphi_2(y)-\varphi_3(z)]dy\,dz, \tag{9}$$

$$A_3(x)\sin\varphi_3(x)=\int\int H(3,3)\cos[\varphi_3(y)-\varphi_3(z)]dy\,dz + \int\int H(2,2)\cos[\varphi_2(y)-\varphi_2(z)]dy\,dz, \tag{10}$$

along with the supplementary condition

$$0=\int\int H(2,1)\sin[\varphi_2(y)-\varphi_1(z)]dy\,dz - \int\int H(2,3)\sin[\varphi_2(y)-\varphi_3(z)]dy\,dz, \tag{11}$$

where

$$H(i,j)=\frac{A_i(y)A_j(z)}{2\pi(1-x^2-y^2-z^2+2xyz)^{1/2}}. \tag{12}$$

Here the region of integration is over the boundary and interior of the ellipse given by $1-x^2-y^2-z^2+2xyz\geqslant 0$. Alvarez-Estrada *et al.* [8] have shown that if

$$\frac{1}{2}\int_{-1}^{1}dx[A_1(x)+A_3(x)]^2<1, \tag{13}$$

then the supplementary condition is already implied by Eqs. (8)–(10) and can be omitted. Equations (8)–(10) are then, in principle, sufficient to obtain the three phase functions ϕ_k. With the inclusion of the supplementary condition, we have an overdetermined system, which in turn puts a stringent constraint on the differential cross-section data. Although the theory described below includes the supplementary condition, our test cases use only Eqs. (8)–(10) as our simulated data are always ‘‘perfect.’’ For real data, the supplementary condition may be useful in obtaining a more accurate result; however, this needs to be investigated in the future.

The solutions of Eqs. (8)–(11) have two discrete ambiguities [8]: (i) The trivial ambiguity where the transformation $\phi_k\rightarrow\pi-\phi_k$, $k=1,2,3$ gives another solution; (ii) if (ϕ_1,ϕ_2,ϕ_3) is a solution, then $(\phi_1,\pi+\phi_2,\phi_3)$ is also a solution.

In order to use Newton's method to solve these four coupled, nonlinear equations, we first rearrange them into operator form, i.e.,

$$F[\Phi]=0, \tag{14}$$

where $\Phi=[\phi_1,\phi_2,\phi_3]$ and 0 is a four-component null vector. This equation can now be solved iteratively as four coupled, linear functional equations using Newton's method, i.e., given Φ^n, Φ^{n+1} is determined according to

$$F[\Phi^n]+F'_{\Phi^n}[\Phi^{n+1}-\Phi^n]=0. \tag{15}$$

Here, F'_{Φ^n} is the Frechet derivative which can be expressed as a 4×3 linear matrix operator acting on ϕ_1,ϕ_2,ϕ_3:

$$F'_1[h_1]=2\int\left\{\int H(1,1)\sin[\phi_1(y)-\phi_1(z)]dz\right\}h_1(y)dy + A_1(x)\cos[\phi_1(x)]h_1(x), \tag{16}$$

$$F'_1[h_2]=2\int\left\{\int H(2,2)\sin[\phi_2(y)-\phi_2(z)]dz\right\}h_2(y)dy, \tag{17}$$

$$F'_1[h_3]=0, \tag{18}$$

$$F'_2[h_1]=\int\left\{\int H(1,2)\sin[\phi_1(y)-\phi_2(z)]dz\right\}h_1(y)dy, \tag{19}$$

$$F_2'[h_2] = \int \left\{ \int H(2,1)\sin[\phi_2(y)-\phi_1(z)] + H(2,3)\sin[\phi_2(y)-\phi_3(z)]dz \right\} h_2(y)dy + A_2(x)\cos[\phi_2(x)]h_2(x), \quad (20)$$

$$F_2'[h_3] = \int \left\{ \int H(3,2)\sin[\phi_3(y)-\phi_2(z)]dz \right\} h_3(y)dy, \quad (21)$$

$$F_3'[h_1] = 0, \quad (22)$$

$$F_3'[h_2] = 2\int \left\{ \int H(2,2)\sin[\phi_2(y)-\phi_2(z)]dz \right\} h_2(y)dy, \quad (23)$$

$$F_3'[h_3] = 2\int \left\{ \int H(3,3)\sin[\phi_3(y)-\phi_3(z)]dz \right\} h_3(y)dy + A_3(x)\cos[\phi_3(x)]h_3(x), \quad (24)$$

$$F_4'[h_1] = \int \left\{ \int H(1,2)\cos[\phi_1(y)-\phi_2(z)]dz \right\} h_1(y)dy, \quad (25)$$

$$F_4'[h_2] = \int \left\{ \int -H(2,1)\cos[\phi_2(y)-\phi_1(z)] + H(2,3)\cos[\phi_2(y)-\phi_3(z)]dz \right\} h_2(y)dy, \quad (26)$$

$$F_4'[h_3] = \int \left\{ \int -H(3,2)\cos[\phi_3(y)-\phi_2(z)]dz \right\} h_3(y)dy, \quad (27)$$

where $h_i = \phi_i^{n+1} - \phi_i^n$. If the integrals over y are approximated by means of a quadrature formula, then Eq. (15) reduces to a system of linear algebraic equations. In the process of solution, it is useful to incorporate a set of limits and a transformation of variables for the two-dimensional integrals in Eqs. (8)–(11) [6].

The iteration procedure starts with initial guesses for ϕ_1, ϕ_2, and ϕ_3. By solving the system of linear equations (15), one obtains a new solution and the process is repeated. If the iteration procedure converges, one obtains an exact solution, although the solution may not be unique. Problems with convergence may arise when any of the ϕ_k have values of $\pi/2$, $3\pi/2, \ldots$ at some points. When this occurs, $\cos\phi_i \to 0$ in some regions and some diagonal elements of F' become very small and the solution to Eq. (15) becomes unstable. This problem is caused by the existence of multiple solutions arising from either of the two discrete ambiguities mentioned previously. In the case of the trivial ambiguity, if ϕ_i, $i = 1,2,3$ is a solution, then $\pi - \phi_i$ is also a solution. The two solutions can only cross at $\pi/2$, $3\pi/2, \ldots$ and the Frechet derivative is close to zero at those points. We also notice that the iteration procedure fails to converge when the Frechet derivative, F', points in the direction of one solution on one interval (say from 0 to θ_t) and toward the other solution on the rest of the interval (from θ_t onward). This particular problem can be overcome by adding a term αI to the Frechet derivative, where I is the identity matrix and α is an adjustable parameter.

In general, in order to achieve convergence, we employed three numerical techniques, each of which involved one parameter. The first technique used singular-valued decomposition (SVD) [9] to solve the linear system of equations (15). The SVD eigenvalues that were smaller than the parameter were truncated to zero. We found that the use of SVD is vital in keeping the iteration stable. The second technique used generalized cross validation (GCV) smoothing [10] where the smoothness was controlled by a parameter. The third technique was to add a term αI to F'_{Φ^n} as mentioned above. This technique was only used when the initial guesses were far from the solution and the inclusion of the term αI could cause the iteration procedure to tend towards the solution. Thus, we used three parameters to control the iteration procedure and the values of these parameters were reduced after each iteration. When the ϕ_i^n were close to the exact solution, the GCV smoothing and the term αI were no longer needed and only the SVD technique was used. All three parameters were initially chosen as small as possible but yet big enough to prevent the iteration process from diverging.

III. RESULTS AND DISCUSSION

As the first test of our iterative method, we used simulated data generated from the parametrized S matrix,

$$S_l = \begin{pmatrix} S_{11} & S_{21} \\ S_{12} & S_{22} \end{pmatrix} = \begin{pmatrix} \eta_l e^{2i\delta_l^{(1)}} & i\sqrt{1-\eta_l^2}\, e^{i(\delta_l^{(1)}+\delta_l^{(2)})} \\ i\sqrt{1-\eta_l^2}\, e^{i(\delta_l^{(1)}+\delta_l^{(2)})} & \eta_l e^{2i\delta_l^{(2)}} \end{pmatrix}, \quad (28)$$

where the quantities $\delta_l^{(1)}$, $\delta_l^{(2)}$ denote the phase shifts and are real; the η_l are the ''elasticities'' and are also real with values ranging between $0 \leqslant \eta_l \leqslant 1$. $\eta_l = 0$ corresponds to completely inelastic scattering, while $\eta_l = 1$ corresponds to the case of pure elastic scattering. The fact that the S matrix is both unitary and symmetrical is a consequence of the conservation of flux and time-reversal invariance, respectively. With the above S matrix, the scattering amplitude for scattering from channel i to channel f is given by

$$f_{fi}(\theta) = \frac{1}{2iK_i} \sum_{l=0}^{\infty} (2l+1)[S_{fi}(l) - \delta_{fi}]P_l(\cos\theta). \quad (29)$$

In this test case, the parameters for the S matrix had the following values:

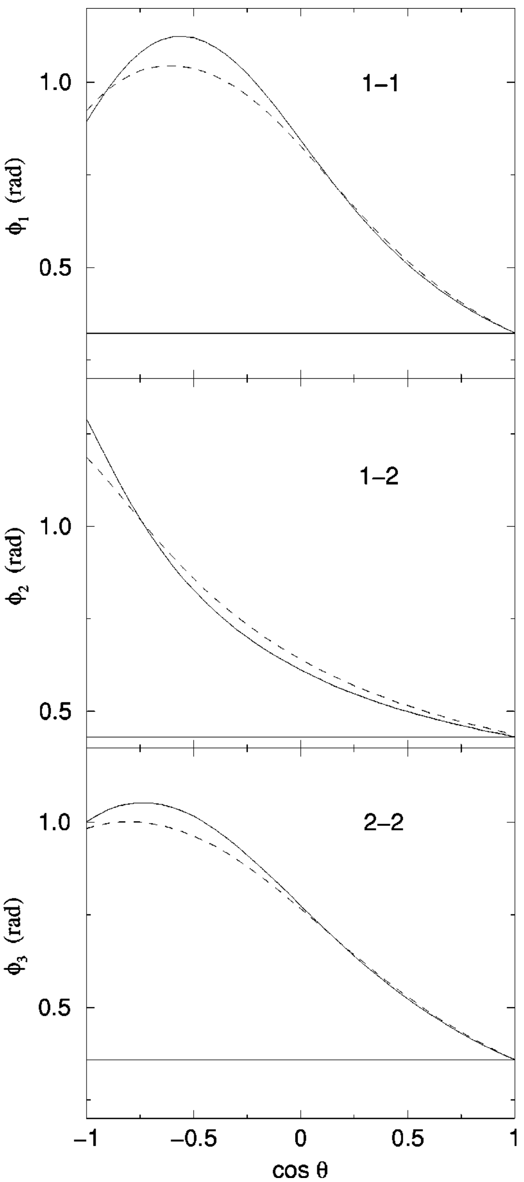

FIG. 1. The solutions ϕ_1, ϕ_2, ϕ_3 of the unitarity equations based upon the simulated data set for two-channel scattering. ϕ_1 is for scattering from channel 1 to channel 1, ϕ_2 for channel 1 to channel 2, and ϕ_3 for channel 2 to channel 2. The horizontal lines are the initial guesses while the dashed lines are the first iterates. The solid lines are the second iterates and the final converged solutions.

$$\delta_0^{(1)}=20° \quad \delta_1^{(1)}=6° \quad \delta_2^{(1)}=2°$$

$$\delta_0^{(2)}=15° \quad \delta_1^{(2)}=4° \quad \delta_2^{(2)}=1°$$

$$\eta_0=0.8 \quad \eta_1=0.99 \quad \eta_2=1.0$$

The initial phase functions were chosen to be constants having the values $\phi_i(\theta)=\phi_i(\theta=0)$. The $\phi_i(\theta=0)$ can be determined from the total cross sections and total elastic cross section. The procedure converged in two iterations without using any of the numerical techniques mentioned above. The results of each iteration are displayed in Fig. 1. From the figure, we can see that after the first iteration the ϕ_i^1 are already close to the exact solution while after the second iteration the ϕ_i^2 cannot be distinguished in the figure from the exact solution.

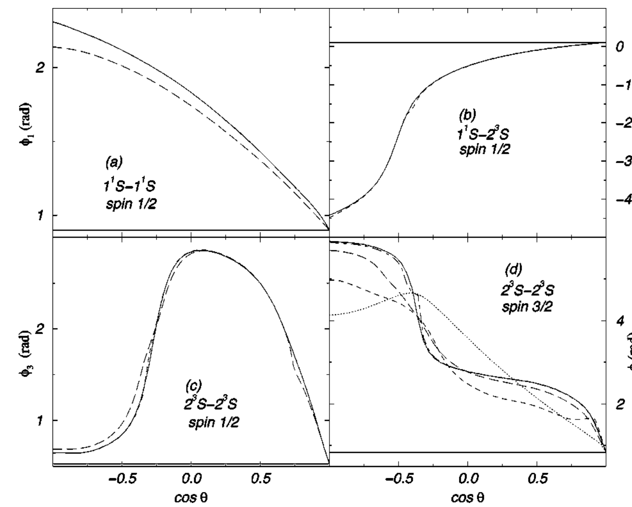

FIG. 2. The solutions ϕ_1, ϕ_2, ϕ_3 of the unitarity equations based upon electron-helium data calculated using the CCC method. (a) ϕ_1 is for the elastic scattering from the ground state. (b) ϕ_2 is for inelastic (doublet) scattering from the ground state to the $2\,^3S$ state. (c) ϕ_3 is for elastic (doublet) scattering from the $2\,^3S$ state. In (a), (b), and (c), the horizontal lines are the initial guesses. The long dashed lines are the solutions of the one-channel approximation (see text). The short dashed lines are the final solution while the solid lines are the exact solution. (d) ϕ is for the one-channel elastic (quartet) scattering from the $2\,^3S$ state. The horizontal line is the initial guess. The dotted, short-dashed, long-dashed, dot-dashed, and solid lines are the 6th, 11th, 16th, 21st, and 26th (exact) iteration results, respectively.

Our second test was the more realistic case of electron-helium scattering. The ground state of helium is the spin-zero singlet state 1^1S. The first excited state is the spin-one triplet state 2^3S at 19.819 eV above the ground state while the second excited state is the spin-zero state 2^1S at 20.615 eV. The electron, of course, has spin-half. We note that elastic scattering from the 2^3S state can give rise to either doublet ($S=1/2$) or quartet ($S=3/2$) scattering. If the input data are the spin-resolved differential cross section ($S=1/2$), we can still use the theory described above, which is for spinless particle scattering. In this test case, the input DCS data were calculated using the convergent close-coupling (CCC) method [11]. The incident electron energy was 20.5 eV and hence 0.682 eV above the first excited state but 0.115 eV below the second excited state. The unitarity equations in this case are more difficult to solve than in the first test. Thus, we made use of the fact that at this scattering energy, the inelastic scattering is very weak compared to the elastic scattering from both the ground state and the first excited state. Consequently, as a first approximation, we could obtain good estimates for ϕ_1 and ϕ_3 by separately applying the one-channel unitarity equation for elastic scattering from the ground and the excited state. With initial guesses of constants, it took 8 and 15 iterations, respectively, of the one-channel unitarity equation for ϕ_1 and ϕ_3 to converge. By using these two one-channel solutions together with ϕ_2^0 equal to a constant as the starting point for the two-channel unitarity equations, we obtained the exact solution after 28 iterations. Since we had set all three initial guesses, ϕ_i^0, to be constants, no *a priori* information about the solution was used apart from determining the constants $\phi_i(\theta=0)$ by the optical theorem, which is a special case of the generalized unitarity theorem. In this test case, we applied all three numerical techniques in order to achieve convergence. The SVD parameter was initially set to 0.1 and then reduced to 0.001 in the last few iterations. Initially the GCV parameter was set to 0.03 while α was chosen to be -0.3 in the term αI. The GCV technique was not used in the last five iterations while the term αI was only used in the first ten iterations. The results for the phase functions are shown in Figs. 2(a)–2(c). We can see that the one-channel approximation brings ϕ_1 and ϕ_3 very close to the exact solution for the two-channel case. The reproduction accuracy obtained here is very good and exceeds typical experimental accuracy. The solution ϕ_1 overlaps with the exact one and the differences cannot be seen from the figure.

For completeness, we also performed a phase-shift analysis for elastic scattering from the 2^3S state which is a one-channel case for the quartet $S=3/2$ differential cross section. By starting with a constant value for the phase function, the Newton iterative method converged after 21 iterations. In this case, we used both the SVD and GCV smoothing techniques in order to achieve convergence. The SVD parameter was initially set to 0.2 and then reduced to 0.1 in the last few iterations while the GCV parameter was initially set to 100 but was only used for the first few iterations. The results for the phase function are shown in Fig. 2(d), where the results from the last iteration are indistinguishable from the exact phase function.

IV. CONCLUSIONS

To conclude, we have developed a procedure to extract the complete scattering amplitude matrix from a complete data set of spin-resolved differential cross sections for two-channel scattering. The generalized unitarity theorem gives rise to a coupled set of nonlinear integral equations for the phase functions of the scattering amplitude elements. A Newton iterative method was used to solve these equations, although additional numerical techniques were needed in order to achieve convergence. This procedure has been successfully used to analyze the doublet differential cross section for electron-helium scattering between the first and second excitation thresholds. It is hoped that experimental data for this case will be available in the near future.

ACKNOWLEDGMENTS

A.P. wishes to thank the people of the Republic of Indonesia for financial support during his studies in Australia. D.R.L. gratefully acknowledges the support of the Australian Research Committee. We also wish to thank Dr. D. V. Fursa for providing us with tabulated data for the electron-helium calculations.

[1] K. Chadan and P. Sabatier, *Inverse Problems in Quantum Scattering Theory*, 2nd ed. (Springer, Berlin, 1989).
[2] R.G. Newton, J. Math. Phys. **9**, 2050 (1968).
[3] A. Martin, Nuovo Cimento A **59**, 131 (1969).
[4] R.B. Gerber and M. Karplus, Phys. Rev. D **1**, 998 (1970).
[5] D. Atkinson, P.W. Johnson, and R.L. Warnock, Commun. Math. Phys. **28**, 133 (1972).
[6] D.R. Lun, L.J. Allen, and K. Amos, Phys. Rev. A **50**, 4000 (1994).
[7] H. Huber, D.R. Lun, L.J. Allen, and K. Amos, Phys. Rev. A **53**, 2015 (1997).
[8] R.F. Alvarez-Estrada, B. Carreras, and G. Mahaux, Nucl. Phys. B **88**, 289 (1975).
[9] *Numerical Recipes*, edited by W.H. Press, B.P. Flannery, S.A. Teukolsky, and W.T. Vetterling (Cambridge University Press, Cambridge, England, 1986), p. 52.
[10] P. Craven and G. Wahba, Numer. Math. **B1**, 377 (1979).
[11] D.V. Fursa and I. Bray, J. Phys. B **30**, 757 (1997).