Analyticity and unitarity as constraints to obtain scattering phase shifts and an application to *e*-He scattering

H. Huber,* D. R. Lun, L. J. Allen, and K. Amos
School of Physics, University of Melbourne, Parkville 3052, Victoria, Australia
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The requirements that the scattering functions for quantal scattering at energies below the first inelastic threshold be unitary and analytic have been used to establish a process that gives the complex scattering amplitudes from differential cross sections. From those amplitudes, scattering phase shifts have been deduced by Legendre integration. The effects of the natural ambiguity of the phase of the scattering amplitude, under conditions for which uniqueness and (numerical) stability of solutions are not assured, also have been studied to show that the process we have developed to specify the scattering phase shifts can give stable nonspurious results. The scattering of electrons from He atoms for incident energies ranging from 1.5 to 19 eV are considered as an example of this procedure. Phase-shift analyses of those data have been made with a variety of other techniques to allow a comparative study of our results and of sets with which are associated fits to cross sections that are statistically significant.
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I. INTRODUCTION

Scattering phase shifts or, equivalently, the scattering (S) functions are central in most analyses of elastic scattering data. They form a link between data, such as differential cross sections, and the interaction potentials between the two scattering particles. That is so if the process of analysis was a direct one, as discussed recently in a review of microscopic model analyses of electron-atom scattering data [1] and of proton scattering from nuclei [2]. It is also the case if one adopts an inverse scattering theory approach, such as in the recent analyses of nuclear heavy-ion scattering, of electron scattering from atoms and molecules and of atom−atom scattering [3]. In direct analyses, the limitations of the many-body model theory used and the approximations needed to make evaluations feasible usually do not lead to quality fits of data. With inversion methods, whether they be of simple numerical type (phenomenological potential parameter fitting) or based upon a formal inverse scattering theory, the processes by which the phase shifts are obtained usually are ambiguous. In numerical inversion, there remain uncertainties such as different potentials giving different sets of phase shifts but equivalent fits to the data, while when formal inverse scattering methods are used, the extraction of the phase shifts as well as their interpolation to all values of angular momenta can be problematic. It is a hope that the conditions of analyticity and unitarity of the S functions can be used to place severe constraints upon such ambiguities, sufficient to ascertain a most physical if not *the* physical set of phase shifts of the scattering process.

Analyticity of the S functions transcribes to a minimal energy path condition for the phase shifts [4] while unitarity leads to the generalized flux theorem [4,5]. Below the first nonelastic threshold and for the scattering of spinless particles (or if one simply ignores any spin-dependent attributes in the scattering), this theorem translates to an integral equation to define the phase, φ, of the scattering amplitude. A solution to that integral equation not only exists, but also, under particular conditions [6], it is unique. Furthermore, with one of those conditions (hereafter defined as the Martin condition) being valid, an iterative method of Newton [5] gives that solution. Of course there is a natural ambiguity due to the unitarity condition, $f(\theta)=-f^{\dagger}(\theta)$, which gives a second solution, a second branch, defined by the phase transform, $\varphi(\theta)\rightarrow\pi-\varphi(\theta)$. The scattering phase shifts, $\delta_{\not/}$, associated with this second solution are simply the negative of those obtained from use of $f(\theta)$. But as we shall show, problems arise in methods of solution for the phase function within the region of intersection of both the actual and the second branch solutions. Those problems can lead to spurious forms for the resultant (calculated) phase function and, therefore, to specification of unphysical phase-shift values. With the Martin condition satisfied, however, no problem exists, as this condition corresponds to scattering from a very weak interaction and/or at very low energies and the associated phase function does not cross the second branch solution.

In cases studied recently [7], the Martin condition was far from being satisfied, and for them a standard fixed-point method of solution [5] of the phase equation did not give a stable result. But another procedure was found with which a stable solution of the phase equation could be obtained. Uniqueness is no longer guaranteed and the phase function can assume large values that may vary through more than one quadrant, so posing questions of (numerical) stability alluded to above. A purpose of this study is to show that analyticity and unitarity can define the (complex) scattering amplitudes up to threshold at least and from which, by Legendre integration, the scattering phase shifts and their variation (with energy) can be specified with or without *a priori*

*Permanent address: Institut für Kernphysik, Technische Universität Wien, Wiedner Hauptstrasse 8-10/142, A-1040 Wien, Austria.

information. By this means we seek to establish the procedures to generate stable, credible scattering amplitudes below threshold, which are needed for us to pursue analyses of data at energies above threshold by solution of the coupled-equations form of the generalized flux theorem [8].

Phase-shift analyses of data are frequently the prelude to specification of an interaction potential between the colliding particles by either use of a specific form of inverse scattering theory or by the more common approach of numerical inversion. With the latter, a form of the interaction is postulated, either purely phenomenologically or predicated upon some underlying theory of the structure of the particles, and then the values of the parameters characterizing the interaction adjusted until an optimal match is found to measured data by using the phase shifts generated to specify the cross section. The typical measure of success is the value of the χ^2 per degree of freedom, χ^2/F. Of the proper inverse scattering theories [4], and of the fixed energy class, some practical success has attended application of the ones in which a rational function form of the S function is assumed [3].

In the next section we briefly review the basic structure of the (scattering amplitude) phase equation and its origin. The results of application to e-He scattering data ranging from 1.5 to 19 eV are then discussed. These data are of high quality and a reliable phase-shift analysis has been done previously [9] with which we compare our results. Also there are theoretical phase shifts calculated with variational methods and with which we can make further comparisons [10].

Our results have been obtained using the method of solution that previously [7] was found to give stable results. In addition, analyticity has been invoked to set the initial phase function guesses for each energy (above 1.5 eV) to be that from the cross-section analysis at the energy immediately below. The effects of the ''natural'' ambiguity, i.e., $\varphi(\theta)\rightarrow\pi-\varphi(\theta)$, are then considered and we show how the existence of two possible solutions can lead to stability problems in seeking a solution, or worse, even spurious solutions of the scattering amplitude phase equation. We define a procedure to prevent such from occurring in the cases studied. Thereafter we compare the phase shifts we have obtained with those from other analyses.

II. UNITARITY AND THE SCATTERING PHASE SHIFTS

As the spin-orbit interaction is weak for the e-He system, we ignore any such effects due to the intrinsic spin of the electron and so express the differential cross sections in terms of scalar scattering amplitudes,

$$f(\theta)=\frac{1}{k}A(\theta)e^{i\varphi(\theta)}, \tag{1}$$

where using $x=\cos(\theta)$,

$$\frac{d\sigma}{d\Omega}=|f(x)|^2=\frac{1}{k^2}A^2(x). \tag{2}$$

The magnitude and phase of those scattering amplitudes may be extracted from the differential cross sections, under the constraint that the scattering function is unitary [5,11], as the generalized unitarity theorem leads to an equation that specifies the phase in terms of the complete (0° to 180°) cross section, viz.,

$$\sin\varphi(x)=\int\int\frac{A(y)A(z)\cos[\varphi(y)-\varphi(z)]}{2\pi A(x)(1-x^2-y^2-z^2+2xyz)^{1/2}}\,dy\;dz,$$

$$=\int\int H(x,y,z)\cos[\varphi(y)-\varphi(z)]\;dy\;dz. \tag{3}$$

Therein the region of integration is the interior of an ellipse.

From the partial-wave expansion of the scattering amplitude,

$$f(\theta)=\frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)e^{i\delta_\ell}\sin(\delta_\ell)P_\ell(\cos(\theta)), \tag{4}$$

the scattering function is obtained by Legendre integration of that scattering amplitude, viz.

$$S_\ell-1=e^{2i\delta_\ell}-1=ik\int_0^\pi f(\theta)P_\ell(\cos(\theta))\sin(\theta)d\theta, \tag{5}$$

which in turn identifies the phase shifts, δ_ℓ.

Solutions of Eq. (3), or its equivalent, have been sought with iteration schemes based on the contraction mapping principle [5,6,11]. That approach also defines an existence condition for a solution and for its global uniqueness as well to be

$$M(x)=\int\int H(x,y,z)\;dy\;dz\leqslant 0.79. \tag{6}$$

In application though there are difficulties. Physical circumstances rarely seem to meet the domain criterion and, without modification of the fixed-point iteration method, stable solutions are not found [12]. Such modification can be made, however [7,12], and stable plausible scattering functions defined. In brief, in that method one considers an operator F that acts upon functions $\varphi(x)$ according to

$$F[\varphi]=\sin[\varphi(x)]-\int\int H(x,y,z)\cos[\varphi(y)-\varphi(z)]\;dy\;dz \tag{7}$$

and its Fréchet derivative, F', which is given by

$$F'_\varphi[h]=\cos[\varphi(x)]h(x)+\int\int H(x,y,z)\sin[\varphi(y)-\varphi(z)]$$
$$\times[h(y)-h(z)]\;dy\;dz$$
$$=\cos[\varphi(x)]h(x)$$
$$+2\int\left(\int H(x,y,z)\sin[\varphi(y)-\varphi(z)]dz\right)h(y)\;dy. \tag{8}$$

This is a bounded linear operator. Then, if one can solve the linear functional equation,

$$F[\varphi^n]+F'_{\varphi^n}[\varphi^{n+1}-\varphi^n]=0, \tag{9}$$

for $\varphi^{(n+1)}$, and if the sequence φ^n converges, its limit is a solution of Eq. (3). Further, if the integral in Eq. (8) is approximated by a quadrature formula, Eq. (9) reduces to that of a linear system. However, the price of finding stable convergent solutions by this means is the loss of guarantee of global uniqueness.

III. APPLICATION TO *e*-He SCATTERING DATA BELOW THRESHOLD

An essential requirement in the use of the generalized flux theorem is to have the differential cross section at all physical scattering angles. With actual data sets this entails both interpolation and extrapolation to specify the input to the method of solution of the phase equation. That process must be ambiguous due at least to the statistical errors always existent with empirical numbers. Additionally, systematic errors can have a considerable impact on what one assesses to be a ''good'' theoretical fit to the data. A recent study [13] has shown that small uncertainties in the assumed scattering angles of the measurements can alter the χ^2 per degree of freedom (χ^2/F) of fits to data significantly (in one of the cases studied [13] by as much as an order of magnitude). We do not consider such systematic errors herein. There remains the systematic errors in magnitudes and these we do consider by using generalized cross validation (GCV) [14] to aid with smoothing of data sets. Thus the interpolation of the current *e*-He data sets of interest has been made by subjecting the measured values to the GCV process to give a ''smoothed'' data set and one that is extended to all physical scattering angles. For the Andrick and Bitsch data [15], that included the extrapolation to 0° and to 180° by taking an additional mesh point at 5° via linear extrapolation of the values at 10° and 15°. The backward angles were set as those given by the spline function resulting from the GCV process. With the data from Brunger *et al.* [9], additional values of the cross sections at 0°, 5°, 140°, 160°, and 180° were calculated from the phase shifts found previously [9]. The GCV methods from the IMSL library utilized *B* splines and in the extrapolation and interpolation of the data, a GCV process of order 11 ensured that the input cross section at all scattering angles was a good fit to the actual data. The GCV process has also been used to smooth variations between iterations of solutions to the phase equations. For this only an order 3 process was required to smooth sufficiently the variation between φ^{n+1} and φ^n. Splines of lower order did not satisfy the (respective) variations well enough. However, despite the resultant cross sections for the smoothing being excellent fits to the measured data sets, in our study of the natural ambiguity we chose to use an artificial cross section at 18 eV. That ideal cross section was obtained by using the rational function form of the *S* function found previously [9] to fit the actual 18-eV data. Therewith we have an ''exact'' phase function to compare with the results of our studies.

Solutions of the nonlinear integral equation for the phase function, $\varphi(\theta)$, were made using the linearizing method [12] and with both a Gauss-Legendre quadrature and a trapezoidal discretization to effect the numerics. Both types of discretization lead to reasonable results in the analysis. But it is crucial to start the ensuing iterations with a reasonable guess at the phase function variation, and to use a smoothing process (GCV) on the phase function changes with each iteration. The need for such a procedure is detailed in the next section with a specific set of results. In the case studied, the variation of the scattering function with energy (analyticity) should not be severe since there are no such special processes (such as sharp resonances) present in *e*-He scattering below threshold. Hence the starting phase function for any calculation is that found from the analysis of the data at the nearest (lower) energy.

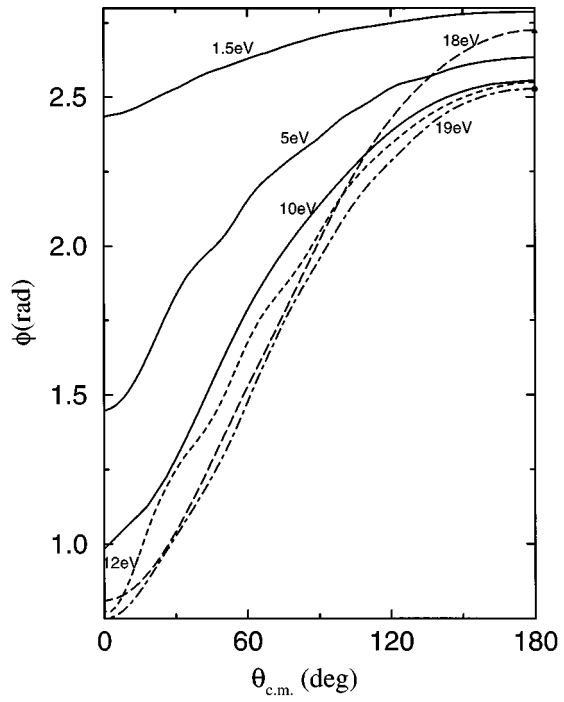

FIG. 1. The phase functions of the scattering amplitudes for the *e*-He scattering for energies as indicated. Each (other than the 1.5-eV result) was obtained by using as input to our method the phase function of the next lowest energy and GCV smoothing was applied at each iterate in the process leading to the final (stable) functions.

The 1.5-eV scattering data satisfy not only the condition [6] for a solution of the phase equation to exist and be unique, but also, as the integral, Eq. (6), is less than $1/\sqrt{2}$ for all scattering angles, the Martin condition is satisfied so that the fixed-point method of solution converges [4]. By this means we have specified the phase function of the scattering amplitude for 1.5-eV electrons off the He atom and then used that as the initial guess to evaluate the 5.0-eV phase equation. As the 5.0-eV and higher-energy data do not satisfy the Martin condition, our method based upon the Fréchet derivatives has been used. The final solutions of the phase equations are plotted in Fig. 1 as functions of the scattering angle. With the 18-eV result being slightly exceptional, there is a smooth trend to these results as energy increases. All of the results are relatively smooth, monotonic functions, which, with the exception of the lowest-energy case, vary from less than 1.5 to near 2.5 rad over the physical range of scattering angles. Thus most of the results cross the natural (second branch) solution of $\pi-\varphi(\theta)$.

With the unitary (complex) scattering amplitudes, $f(\theta)$, thereby completely defined, we have obtained the (real) scat-

tering phase shifts from solutions of Eq. (5). Then by forming the partial-wave summations of Eq. (4) to reform a scattering amplitude and cross section, we obtained the results shown by the solid curves in Figs. 2 and 3. In the first of these diagrams the results for the 1.5-, 5-, and 10-eV set of calculations are compared with the data and with the cross sections found by an alternative search procedure (dashed curves), which are discussed later. Likewise the 12-, 18-, and 19-eV results are compared in Fig. 3 with the data and the results from an alternative search procedure. As they should be, the fits to the data are excellent.

IV. EFFECTS OF THE ''NATURAL'' AMBIGUITY

One goal of our investigations was to assess the influence of the ''natural'' ambiguity, viz. $\varphi \rightarrow \pi - \varphi$, upon numerical solutions of the nonlinear phase equations for actual scattering cases. We have found that this can result in numerical instabilities within the crossing region of both solutions or to spurious solutions as an extreme form by using a small mesh size discretization.

These studies also emphasize the value of using analyticity in the analyses reported above. At the lowest energy considered, the Martin condition was satisfied by the cross section at all scattering angles, so the solution to the phase equation was not only unique but could be found by using the Newton fixed-point method. The Martin condition ensures that this solution and the natural ambiguity (second branch) solution do not intersect.

A. Numerical stability

A numerical problem can arise if values of φ lie near to $\pi/2$ as then so also do values of $\pi - \varphi$. This is evident when one considers the integral equation for the phase function in the form

$$\sin(\varphi(x)) = \int \int H(x,y,z)\cos[\varphi(y) - \varphi(z)]\, dy\, dz, \tag{10}$$

from which it can be seen that the overall transform $\varphi \rightarrow \pi - \varphi$ gives a second solution. But any combination of both (i.e., a ''branch flip'' with some values of φ on the first branch and others on the second) is not another solution to the integral equation. However, within the intersection region, such branch flips may occur in a numerical solution formed from the algebraic system [12] we use to evaluate the integrals. That we can see by considering the cosine term in the integral, in the standard expansion,

$$\cos[\varphi(y) - \varphi(z)] = \cos[\varphi(y)]\cos[\varphi(z)] + \sin[\varphi(y)]\sin[\varphi(z)]. \tag{11}$$

When values of $\varphi(z)$ or $\varphi(y)$ (or both) are close to $\pi/2$, the first term on the right-hand side is negligible while the second one is invariant under the transform $\varphi(y) = \pi - \varphi(y)$ and/or $\varphi(z) = \pi - \varphi(z)$. As a consequence, in such a region, the contributions to integrals from either branch solution being used in a numerical evaluation are nearly identical. Then the (numerically specified) phase function is very sensitive to the accuracy of evaluation of the integral, and branch flips may result due to a slight variation of the numerical value from the exact result. Further, and as a consequence of the discretization of our method, the exact values of the phase function may be determined only at the fixed values of the mesh points. Interpolation of those values must then be made to find the (more) complete phase function as needed to evaluate the integral in Eq. (10). Initially, a cubic spine method was chosen to effect this. Consequently, the exact value of the integral will never be known precisely. With the left-hand side of Eq. (10) being invariant under the specified transform, such (small) systematic inaccuracy, coupled with the high sensitivity of the linearized equations for the integral in those regions, are the cause why solution of the dis-

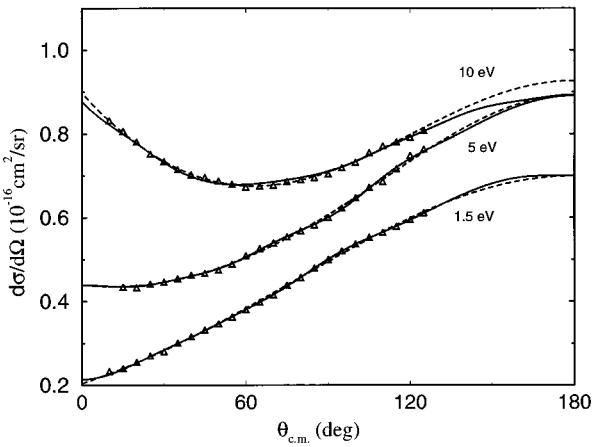

FIG. 2. The cross sections for 1.5-, 5-, and 10-eV electrons found using the phase shifts extracted by Legendre integration of the scattering amplitudes defined by the phases given in Fig. 1 compared with the data [9]. Those results are displayed by the solid lines, while those portrayed by the dashed curves are the result of using the Search 2 set of phase shifts. The 5- and 10-eV results have been uniformly increased by 0.2 and 0.4 $Å^2$/sr to facilitate viewing.

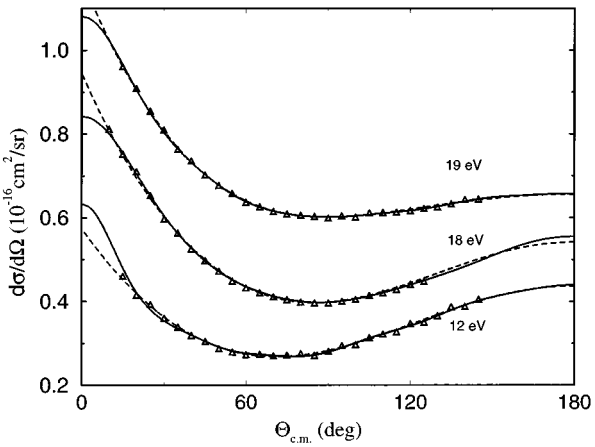

FIG. 3. The cross sections for 12-, 18-, and 19-eV electrons found using the phase shifts extracted by Legendre integration of the scattering amplitudes defined by the phases given in Fig. 1 compared with the data (18 eV from Ref. [9] and 12 and 19 eV from Ref. [15]). Those results are displayed by the solid lines, while those portrayed by the dashed curves are the result of using the Search 2 set of phase shifts. The 18- and 19-eV results have been uniformly increased by 0.2 and 0.4 $Å^2$/sr to facilitate viewing.

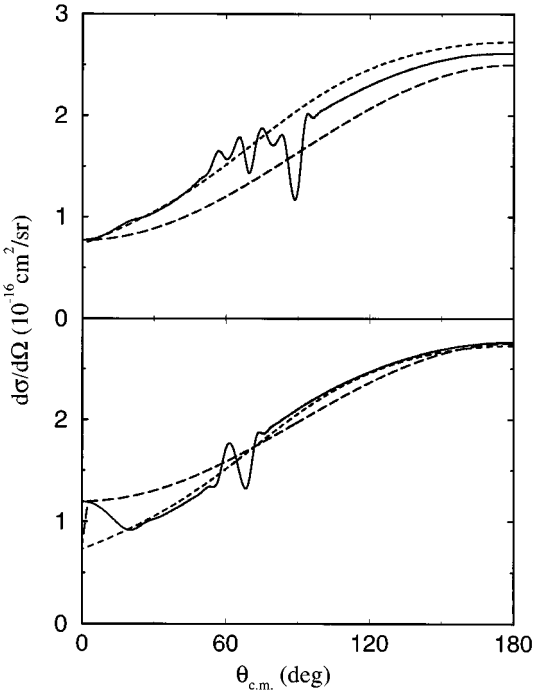

FIG. 4. The phase functions of the 18-eV test calculation found without use of GCV on each iteration with the straight-line initial conditions as detailed in the text. The ''exact'' values are displayed by the small dashed curves, the initial phase functions, $\varphi^{(0)}(\theta)$, by the long dashed curves, and the solutions of the integral equation by the solid curves.

cretized version of Eq. (8) may have branch flips in each iterate at certain mesh points. Interpolation of any such iterate set of values for $\varphi_n(x)$ then can lead to a strong oscillatory behavior of the continuous $\varphi_n(x)$ and, thus, to a significantly different value for the integral (from its true one) in the next step of the iteration process.

To demonstrate this problem, and to indicate a procedure to avoid it, we have considered the cross section evaluated with the rational S function fit to the 18-eV e-He scattering data [9] as the ''data'' at all physical scattering angles. Thereby we have the exact phase function, $\varphi(\theta)$, of the scattering amplitude with which to compare the results of calculations. Our initial guesses for the phase functions were

$$\varphi(\theta)=\phi_0+\frac{1+\cos(\theta)}{2}(\phi_m-\phi_0), \tag{12}$$

where ϕ_0 and ϕ_m are adjustable. The results are shown in Fig. 4 for different initial conditions, with the solid curves portraying the end result, the long dashed curves the initial phase functions, and the small dashed curves the ''exact'' values. The results given in the top section of this diagram were obtained using ϕ_0 (ϕ_m) values of 0.77 (2.5) while those shown in the bottom section were found when the process started with the values 1.2 (2.7). In both results, branch effects centered about the angular region where $\varphi\sim\pi/2$ are evident, but both results tend to the ''exact'' ones. The results in the bottom section are in quite good agreement with the ''exact'' phase function for most scattering angles with but a slight variation occurring in the values for $\theta\approx 60°$. As

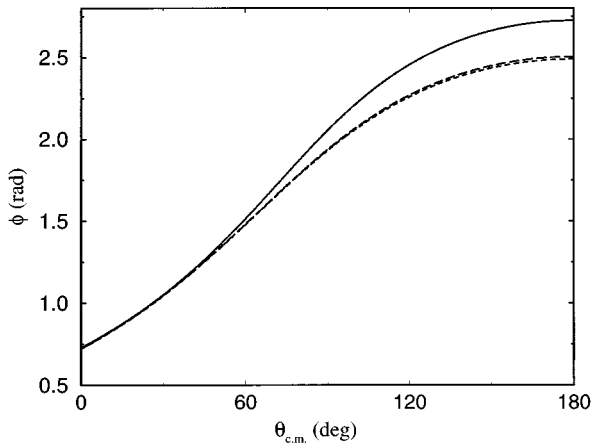

FIG. 5. The scattering amplitude phase functions associated with the three model analyses of the 18-eV e-He differential cross sections shown in Fig. 6

the initial conditions are chosen further removed from the shape of the ''exact'' result, these variations become more pronounced. We repeated these calculations adding a GCV smoothing of the differences between the iterates at each step, and in all cases the final solutions were then excellent reproductions of the ''exact'' phase function. GCV smoothing of the changes with iteration specifically changes the current iterate phase-shift function to be less radically varied from the preceding iterate while remaining as ''faithful'' as possible to the actual calculated iterate function. Thus smoothing of the phase function between iterations, by using generalized cross validation on the differences between the nth and $(n+1)$th iterates, prevents branch flips, but one must start the iterative procedure with a reasonable choice for the phase function to ensure a stable result.

As a second study of the effects of the initial guess of the phase function, we chose the values given by using the phase shifts of the variational model of Nesbet [10] and by the analysis of Williams [16] for the 18-eV data. They are shown by the long and short dashed curves, respectively, in Fig. 5 and therein they are compared with the ''exact'' result sought (solid curve). The cross sections associated with these two model forms are given in Fig. 6, from which it is clear that they are not in very good agreement with the 18-eV data of Brunger *et al.* [9]. However, by using the ''exact'' cross section in the unitarity equation, after but a few iterations the ''exact'' phase variation results with either model starting function. Consequently both the Nesbet and Williams phase shifts are not ambiguous solutions to the generalized flux equation, rather they are just less adequate representations of this 18-eV data (than the rational S function specification).

B. Spurious solutions

If one starts with a phase function quite removed from the exact solution, depending upon the care taken with numerics (i.e., without smoothing and using low mesh sizes), another solution is feasible. At each angle the phase function attempts to converge to the closest branch [$\varphi(\theta)$ or $\pi-\varphi(\theta)$] and the error caused by the solution in any region being on the second branch is compensated by oscillations in

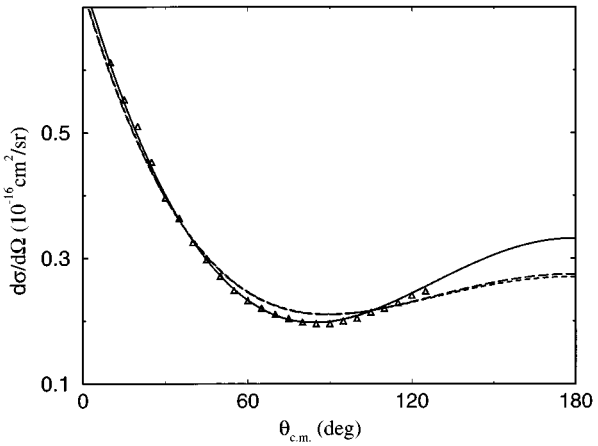

FIG. 6. Fits to the 18-eV e-He scattering data [9] obtained using a (two-pole pair) rational S function [9] (solid curve), using the variational model [10] (long dashed curve) and using the Williams phase shifts [16] (small dashed curve).

the phase function elsewhere. This can be seen as an extreme form of the branch effects discussed in Sec. IV A. In this case, the resulting phase function is nearly symmetric because the crossing point of the two branches is close to $\pi/2$.

Again, we consider the schematical 18-eV e-He scattering with the phase shifts obtained from the rational fit to the data using two starting phase functions. The first is the straight line, $\varphi^{(0)}(\theta)=0.764$, and the second, a shifted Lorentzian,

$$\varphi^{(0)}(\theta)=\frac{0.5}{\cos^2(\theta)+0.25}+0.364. \tag{13}$$

Without smoothing between each iteration and using a 20-(18-) mesh-point quadrature for the constant (Lorentzian) initial condition, solutions as shown in Fig. 7 were obtained. Therein the dashed curve is the result found with the straight-line initial condition and the solid curve that from the Lorentzian one. Not only do these two results differ, but they are also very far removed from an exact solution. These functions lead to radically different phase shifts when Legendre integrations of the complex scattering amplitudes are made. Moreover, since the resulting phase of the scattering amplitude is nearly symmetric, the phase shifts corresponding to odd values of the angular momentum ℓ are small and the underlying quantum interaction would be parity dependent. But these solutions are spurious. When a larger mesh was used, convergence was not achieved. The spurious solution has led to local minima in the root-finding method that stops the process from reaching the proper stable result.

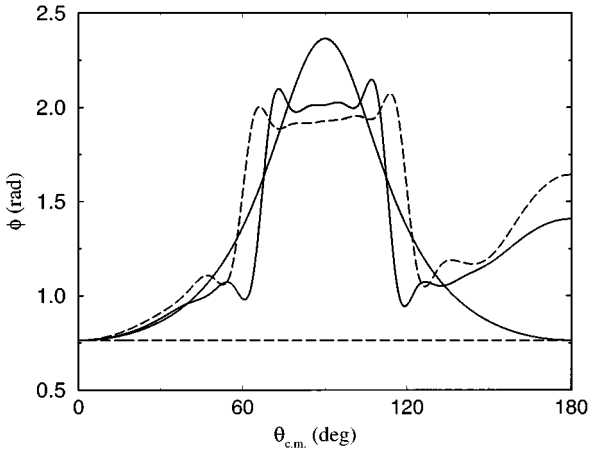

FIG. 7. The phase functions of the scattering amplitude for 18-eV e-He scattering found using the straight line and shifted Lorentzian initial guesses.

V. COMPARISON OF THE RESULTS OF PHASE-SHIFT ANALYSES

The asymptotic (large radius) behavior of the interactions promoting most quantum (elastic) scattering events is known, and as a consequence, so then is the behavior of the scattering phase shifts for large partial waves. For interactions that behave asymptotically as $r^{-(n+1)}$, the phase shifts must vary (asymptotically) as ℓ^{-n} [4]. Thus as the long-range character of the e-He interaction varies as r^{-4}, the scattering phase shifts will vary as ℓ^{-3}. For low energies, in addition, by using an effective range (r_0) approximation, O'Malley *et al.* [17] have shown that, when the energies satisfy $k^{-1}<r_0$, the r^{-4} potential leads to a phase-shift variation

$$\delta_\ell \approx \tan\delta_\ell \approx \frac{\pi k^2 \alpha}{(2\ell+3)(2\ell+1)(2\ell-1)}, \quad \ell>0. \tag{14}$$

Therein α is the dipole polarization. Further, if this variation is valid for partial waves $\ell>N$, by using Thompson's formula [18], the scattering amplitude from Eq. (4) can be written in closed form, viz.

$$\begin{aligned} f(\theta)=&\frac{1}{k}\sum_{\ell=0}^{N}(2\ell+1)e^{i\delta_\ell}\sin(\delta_\ell)P_\ell(\cos(\theta)) \\ &+\pi\alpha k\left[\frac{1}{3}-\frac{1}{2}\sin\left(\frac{\theta}{2}\right)\right. \\ &\left.-\sum_{\ell=1}^{N}\frac{1}{(2\ell+3)(2\ell-1)}P_\ell(\cos(\theta))\right]. \end{aligned} \tag{15}$$

For electron scattering from He atoms with energies up to threshold (19.2 eV), N can be chosen as 1 or 2 in the above, and so Eq. (15), with the dipole polarization taken as 1.38 a.u., can be used with δ_0, δ_1, and perhaps δ_2 as free parameters to be optimized by a χ^2 minimization fit to the available scattering data. Using the nonlinear fitting program, E04FB4, contained in the NAGLIB library and based upon the Marquardt algorithm, the phase shifts so determined against the data of Brunger *et al.* [9] and of Andrick and Bitsch [15] are given in Tables I and II, wherein they are compared with the assessments of others. Therein we display the first four phase shifts determined by the fit searches identified as ''Search 1'' when δ_0 and δ_1 were varied and with the O'Malley phase shifts, Eq. (14), for other partial waves (values listed in the ''expansion'' column of the tables), and by ''Search 2'' when δ_2 is also a free parameter. The attendant χ^2/F values of the Search 1 (Search 2) fits are 0.57(0.62), 2.93(1.80), 1.35(1.16), 1.43(1.43), 3.82(1.16),

TABLE I. Phase shifts from various analyses of the e-He cross sections from Ref. [9].

	ℓ	Search 1	Search 2	Rational fit [a]	Unitarity	Expansion
E=1.5 eV	0	2.6939	2.6939	2.691	2.6937	
	1	0.0393	0.0393	0.0391	0.0397	
	2		0.0046	0.0049	.0044	0.0046
	3			0.0016	.0016	0.0015
E=5 eV	0	2.3469	2.3463	2.346	2.3472	
	1	0.1239	0.1244	0.123	0.1234	
	2		0.0118	0.0123	0.0132	0.0152
	3			0.0040	0.0060	0.0051
E=10 eV	0	2.0885	2.0845	2.0840	2.0746	
	1	0.2380	0.2357	0.2330	0.2204	
	2		0.0286	0.0315	0.0336	0.0304
	3			0.0104	0.0137	0.0102
E=18 eV	0	1.9636	1.9488	1.946	1.9288	
	1	0.3684	0.3627	0.359	0.3536	
	2		0.0505	0.0529	0.0475	0.0548
	3			0.0180	0.0225	0.0186

[a]Reference [9].

and 2.27(1.91) for each energy in increasing order, respectively. The data at 1.5, 5, 10, and 18 eV were those of Brunger *et al.* [9] and had been analyzed assuming a rational function form for the scattering S matrix; a form convenient to effect (WKB) inversion and so define an e-He interaction potential in coordinate space. At 12 and 19 eV, the data were measured by Andrick and Bitsch [15] and the results of our searches are compared with those found from a first-principles variational model calculation [10] as well as by a phase-shift analysis by Williams [16] but of a different data set, one should note. These search and model calculation phase shifts are compared at all energies with the results we have found by using unitarity and analyticity to extract the scattering amplitudes from the measured data and then performing the appropriate Legendre integrations. Clearly all s-wave phase shifts match to within a percent. The p-wave phase shifts vary a little more, with agreement to within 5% in the case of 12 eV. The d-wave values are quite small but even so all analyses concur to within 5% again.

However, disagreement between phase-shift sets in some cases is reflective of the different data sets used in the analyses. At 5.0 eV, the Brunger *et al.* [9] and Andrick and Bitsch [15] data sets are slightly different, the former being a few percent smaller overall than the latter. This is evident in Fig. 8, wherein the two data sets are compared with the cross sections found with our unitarity based set of phase shifts (solid curve) for the Brunger *et al.* data (dots) and the calculation of Williams (dashed curve) with the data of Andrick and Bitsch (open triangles). Brunger *et al.* limit their total error to the range 3.5–5 %, while Andrick and Bitsch assign a systematic error of 3–4 % with a statistical error of 0.5–1.5 %. Clearly the results of analyses of the two data sets cannot be in agreement to the extent one would like.

Finally the d- and f-wave phase shifts found from the unitarity analyses are compared with the O'Malley approximation forms for the e-He dipole polarization interaction. The agreement between these small values is quite good but there is some variation between the formula values [from Eq. (15)] and the unitarity based results with both energy and increasing partial waves. That is evident from Figs. 2 and 3 in which the data are compared with recalculated cross sections; i.e., with cross sections calculated using the tabulated phase shifts. Using the Search 2 phase shifts gave the results portrayed by the dashed curves therein. Recall that the solid curves were obtained using the phases shifts found by using unitarity and analyticity to specify the scattering amplitudes.

TABLE II. Phase shifts from various analyses of e-He cross sections taken from Ref. [15].

	ℓ	Search 1	Search 2	Nesbet [a]	Williams [b]	Unitarity	Expansion
E=12 eV	0	1.9968	1.9919	1.9919	1.9891	1.9856	
	1	0.2577	0.2541	0.2433	0.242	0.2506	
	2		0.0362	0.0365	0.0372	0.0357	0.0365
	3					0.0105	0.0122
E=19 eV	0	1.8256	1.8219	1.8034	1.800	1.8227	
	1	0.3315	0.3251	0.3158	0.311	0.3233	
	2		0.0626	0.0578	0.058	0.0629	0.0578
	3					0.0209	0.0193

[a]Reference [10].
[b]Reference [16].

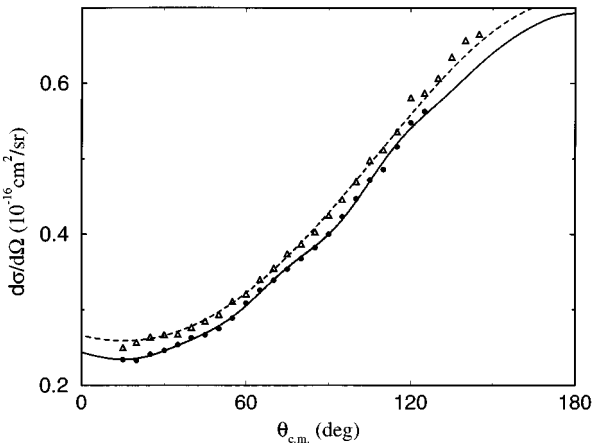

FIG. 8. Comparisons of the 5-eV *e*-He differential cross sections measured by Andrick and Bitsch [15] (open triangles) and of Brunger *et al.* [9] (dots) with the calculated results found by using Williams [16] phase shifts (dashed curve) and those from our unitarity based study (solid curve).

Clearly by taking the asymptotic potential and its high-partial-wave phase shifts *a priori*, the calculated cross sections are smoother than the data, while the unitarity defined set, being ''controlled'' by the actual measured data in the first place, has tried to reproduce the shape minutiae of the variation in the observations. That is especially obvious with the 5-eV results.

VI. CONCLUSIONS

The mathematical requirements that the elastic scattering *S* function for scattering at energies below the first nonelastic threshold be unitary and analytic, have been used to determine the (complex) scattering amplitudes from the cross sections. Application has been made to specify those scattering amplitudes for electrons scattered from He atoms with energies between 1.5 and 19 eV. The unitarity requirement, the generalized flux theorem, transcribes to a nonlinear integral equation for the phase function of the scattering amplitude, the solution of which entails knowledge of the cross sections for all physical scattering angles. The lowest-energy data considered, at 1.5 eV, satisfies a basic condition, the Martin condition, at all scattering angles. Consequently, a solution of the associated integral equation not only was known to exist but also that solution was defined to be unique and could be specified by a fixed-point method of solution. Such was done and the result used as the initial trial solution in our attempt to obtain a solution for the scattering at the next energy (5 eV) at which scattering data existed. At that and higher energies, the data did not satisfy the Martin condition at all scattering angles and the fixed-point method of solution was no longer a stable one. However, another method of solution gave stable results and its use led to accurate candidate phase functions from which, by Legendre integration of the associated scattering amplitudes, real scattering phase shifts were derived. Use of those phase shifts in the partial-wave summations to respecify the cross sections confirmed that the sets gave statistically significant fits to the actual measured data. Of significance was the use of the analyticity of the scattering amplitudes. Thereby a solution at one energy provided the initial guess for our method to converge to a sensible result at the next (higher) energy.

We have studied the effects of the natural ambiguity, namely that the function, $\pi-\varphi(\theta)$, is also a solution, upon the numerical solution of the nonlinear integral equations. In the cases considered, at all energies except the lowest for which data the Martin condition is satisfied, the second branch's solution intersected with the ones sought. Numerically then, at scattering angles around the crossing point, either solution may be the result, and that ambivalence led to calculated results containing oscillations when monotonic phase functions were the actual solutions. In the extreme case, a quite spurious solution function could be the result. But, by using a smoothing procedure upon the rate of change between iterations in the solution method, we were able to prevent branch flips. In the cases studied the generalized cross validation smoothing process was used.

The sets of phase shifts we have obtained were compared with those from other studies of these scattering data, and were found by various data fit procedures or from model potential scattering calculations. Differences have been noted, but they seem to be more a reflection of the differences between the actual data sets used in those studies than of inadequacies of one method of analysis compared to another.

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