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Reconstruction of the potential from scattering data

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We propose an efficient method for reconstruction of the potential from scattering data. Starting from experimentally determined phase shifts and taking into consideration the incompleteness and inexactness of the input information, we construct iteratively a local potential that approximates the input phase shifts. The method is first tested on model examples and is then used for construction of a local effective potential describing the scattering of low-energy electrons by noble-gas atoms. Convergence of the method is usually very fast, and the reconstructed potential is close to the true one. A relation between the inverse-scattering problem and the Fourier analysis of experimental data is discussed.

I. INTRODUCTION

It is well known that, for a solution of the inverse-scattering problem by the classical approaches of Gelfand and Levitan,[1] Marchenko,[2] or Newton,[3] one requires a knowledge of either all the phase shifts at one energy or of one phase shift at all energies together with the energies of any bound states and their normalization coefficients. Obviously, such complete information can never be obtained from experiment. Usually only a finite set of phase shifts at discrete energies, measured with an (often large) error, is available. All practical methods for construction of the potential from experimental data must take into account the fact that the input information is incomplete and inexact. The classical Gelfand-Levitan-Marchenko methods are inappropriate for this purpose. The commonly accepted way of avoiding such problems is to construct a model analytic potential and to fit its parameters to the experimental data by the least-squares method. In most cases only the Woods-Saxon potential has been used to construct a nuclear optical potential. This approach has several shortcomings: (i) lack of uniqueness; (ii) the quality of the fit is not always satisfactory; (iii) a relative complexity and inconvenience of the whole procedure which fits simultaneously many nonlinear parameters; (iv) lack of correlation of the parameters obtained at various energies; etc.

A detailed analysis of these shortcomings leads us to the development of an efficient inversion method that is largely free of such drawbacks. The method is linear, i.e., no nonlinear minimization procedure is used, and at each step in the construction of the potential only a simple system of linear equations of low dimension must be solved. The method is iterative and usually rapidly convergent. The potential is assumed to belong to a class of "reasonable" functions (see the following), but no specific form of the potential is assumed in advance. The uniqueness of the constructed potential depends of course on the class of functions selected to represent the potential, on the starting approximation to it, on the input data set, etc. Moreover, experimental data at various energies and different partial waves are used simultaneously and, what is most important, the method is closely related to the Fourier expansion of the interaction potentials in scattering wave functions. This fact makes it possible to relate the uncertainty of the constructed potential to the incompleteness and inaccuracy of the experimental data. Recently several practical approaches have been proposed for solving the inverse-scattering problem with realistic input data. The most important among them are probably the method of inverting the potential at one fixed energy developed by Mackintosh and co-workers,[4] which is closely related to our approach, namely the method of Lipperheide *et al.*,[5] that of von Geramb,[6] Münchow and Scheid,[7] and very recently by Staszewska.[8]

The purpose of the present paper is to study the general properties of the inversion scheme rather than to carry out the inversion procedure for realistic data.

The method of inversion is described in Sec. II. Section III is devoted to a comprehensive test of the method for a simple potential. A relation with Fourier analysis is established, and error bars are estimated. In Sec. IV the method is used to invert model data representing elastic scattering of electrons on noble-gas atoms.

II. INVERSION METHOD

In this paper we shall discuss the problem of constructing a local energy-independent potential that reproduced given phase shifts with a prescribed accuracy. In general, such a problem may have no solution because the input data set may be inconsistent. In practice there is no reason to use only data at one fixed energy or a fixed angular momentum for the reconstruction of the potential since such input data may not contain all the information required for the unique reconstruction of the potential. This is so because the phase shifts at high energies E and large values of angular momentum l cannot be determined accurately from experiment. For simplicity we restrict our discussion to real phase shifts and real potentials. The inverse-scattering problem with complex potentials will be considered separately. As we have already stated, we use, in contrast to the classical approaches, all available experimental information. As the input information, we use all the known phase shifts, i.e., the available phase shifts at all l and E. This makes the method of inversion more reliable. In the following we shall denote the experimental phase shifts by δ_k^{expt}, where the single subscript k labels the phase shifts at various energies E and various momenta l. We shall represent the required local potential in the form of the expansion in a class of "reasonable" functions (e.g., in the class of functions having all derivatives and decreasing sufficiently rapidly at infinity, etc.)

$$V(r) = \sum_{i=1}^{N} c_i \varphi_i(r) \ . \tag{1}$$

If the functions $\varphi_i(r)$ form a complete set of orthonormal functions, the coefficients c_i are the Fourier coefficients of the unknown potential $V(r)$:

$$c_i = \int V(r)\varphi_i(r)dr \ . \tag{2}$$

Hence, to solve our problem we must find the coefficients c_i that minimize the sum

$$\chi^2 = \sum_{k=1}^{M} [\delta_k(c_i) - \delta_k^{\text{expt}}]^2, \quad M \geq N \ . \tag{3}$$

Here, $\delta_k(c_i)$ denote the phase shifts calculated with the potential (1), and the sum runs over all energies and partial waves available; M is the total number of experimental points.

Clearly, the minimum of χ^2 [Eq. (3)] will decrease to zero with increasing number N of terms in the expansion (1), provided the solution exists and lies in the space spanned by the functions $\{\varphi_i\}$. In the vicinity of a minimum, say, at the point $\{c_i^{(0)}\}$, we can employ a simple linear algorithm[9] for finding a better approximation to the parameters $\{c_i\}$. This algorithm has been widely used in the least-squares methods and consists in retaining only the linear terms in the expansion

$$\delta_k(c_i) \approx \delta_k(c_i^{(0)}) + \sum_i \frac{\partial \delta_k}{\partial c_i}\Bigg|_{c_i = c_i^{(0)}} (c_i - c_i^{(0)}) \ . \tag{4}$$

To minimize χ^2 we set the derivatives of χ^2 equal to zero:

$$D_j(c_i) \equiv \frac{\partial \chi^2}{\partial c_i} = 2\sum_k [\delta_k(c_j) - \delta_k^{\text{expt}}]\frac{\partial \delta_k}{\partial c_i} = 0 \ . \tag{5}$$

Retaining only the linear terms in the expansion of δ_k, we arrive at a system of linear equations for the increments $\Delta c_i = c_i - c_i^{(0)}$:

$$2\sum_k \left[\delta_k^{(0)} + \sum_j \frac{\partial \delta_k^{(0)}}{\partial c_j}\Delta c_j - \delta_k^{\text{expt}}\right]\frac{\partial \delta_k^{(0)}}{\partial c_i} = 0$$

with

$$\delta_k^{(0)} \equiv \delta_k(c^{(0)}) \ .$$

This system can be written as

$$\sum_j A_{ij}\Delta c_j = -D_i \ , \tag{6}$$

where

$$A_{ij} = 2\sum_k \frac{\partial \delta_k}{\partial c_i}\frac{\partial \delta_k}{\partial c_j} \tag{7}$$

and the derivatives are taken at the point $c_i^{(0)}$.

The matrix A, the so-called covariance matrix, is a symmetric positive-definite matrix approximating the matrix of the second derivatives of χ^2:

$$A_{ij} \approx \frac{\partial^2 \chi^2}{\partial c_i \partial c_j} \ .$$

For the system of linear equations (6) to have a solution, the number of experimental points M must exceed the number of parameters, i.e., $M \geq N$. It is worth noting that the exact matrix of the second derivatives of χ^2 is equal to the sum

$$\frac{\partial^2 \chi^2}{\partial c_i \partial c_j} = A_{ij} + 2\sum_k (\delta_k - \delta_k^{\text{expt}})\frac{\partial^2 \delta_k}{\partial c_i \partial c_j} \tag{8}$$

and, if the minimum of χ^2 is equal to zero, i.e., $\delta_k = \delta_k^{\text{expt}}$, this matrix coincides with A_{ij}. In other words, those solutions that lead to small absolute values of χ^2, i.e., that yield an accurate solution of the inverse-scattering problem, can always be found by the linearized algorithm described above.

The phase shift is determined in terms of the real angular solution ψ_l of the Schrödinger equation

$$\left[\frac{\hbar^2}{2m}\left[-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2}\right] + V(r) + V^c(r) - E\right]\psi_l(p,r) = 0 \tag{9}$$

as

$$\tan\delta_l(p) = -\frac{2m}{\hbar^2 p}\int F_l(pr)V(r)\psi_l(p,r)dr \ . \tag{10}$$

The regular solution $\psi_l(r)$ is normalized as

$$\psi_l(p,r) \underset{r\to\infty}{\sim} F_l(pr) + \tan\delta_l G_l(pr) \ , \tag{11}$$

where F_l and G_l are the regular and irregular wave functions of the Coulomb potential $V^c(r)$.

If $V^c = 0$, then $F_l = j_l(pr)$ and $G_l = n_l(pr)$. The derivatives of the phase shifts with respect to the parameters c_i can be easily obtained from Eq. (10):

$$\frac{\partial \delta_l}{\partial c_i} = -\frac{\cos^2\delta_l}{p}\frac{2m}{\hbar^2}\int \psi_l^2(p,r)\frac{\partial V(r)}{\partial c_i}dr \ . \tag{12}$$

This is an analog of the Hellman-Feynman theorem for the case of the continuum spectrum. As a result, the derivatives of the phase shifts are easily calculated simultaneously with the solution of the Schrödinger equation.

Summarizing, the proposed algorithm is defined as follows.

(1) A starting approximation $V^{(0)}(r)$ is chosen:

$$V_{(r)}^{(0)}=\sum_{i} c_i^{(0)}\varphi_i(r) .$$

(2) The phase shifts and their derivatives are computed for this potential.

(3) After constructing A_{ij} and D_i, Eq. (5) is solved and a new improved potential

$$V_{(r)}^{(1)}=\sum_{i}(c_i^{(0)}+\Delta c_i)\varphi_i(r)$$

is generated.

Steps (2) and (3) are repeated until one of the following conditions is satisfied:

$$\text{(i)}\quad |\chi_{n-1}^2-\chi_n^2|<\epsilon ,$$

$$\text{(ii)}\quad \left[\sum_{i=1}^{N}(\Delta D_i)^2\right]^{1/2}<\epsilon ,$$

$$\text{(iii)}\quad \left[\sum_{i=1}^{N}(\Delta c_i)^2\right]^{1/2}<\epsilon .$$

Here, χ_n^2 denotes the current value of χ^2 at the nth iteration. The rate of convergence of this scheme depends on the initial input data set (its completeness and consistency), on the choice of the basis functions $\{\varphi_i\}$, and on the starting approximation $\{c_i^{(0)}\}$. As a rule, if the iteration process converges, its convergence rate is very fast, and 3–5 iterations usually yield converged results.

The proposed method therefore comprises the following elements: (1) decomposition of the potential in a complete basis; (2) determination of the derivatives of the phase shifts by means of Eq. (12); (3) the linearized procedure for minimizing χ^2; and (4) the iterations.

It is this combination of all these elements that makes it possible to construct accurately a potential for all types of input information (given one partial phase shift at a number of energies, all partial-wave phase shifts at one energy, or any combination of input information), provided the input information is sufficient for reconstruction of the potential.

If the input information is not sufficient for precise reconstruction of the potential, it is possible to relax the condition of the completeness and to retain only a few terms (say 1–3) in expansion (1). Then the solution obtained is unique on the restricted basis space. Equation (12) greatly reduces the computational effort required and serves as a basis for the linearization of the χ^2 minimization. This linearized iterative approach to the minimization permits a rapid determination of a minimum with a very small function value even in the case of a very large number of variables. It is very difficult and time consuming to find such a minimum by general nonlinear minimization methods.

III. MODEL POTENTIALS

To gain insight into the efficiency of our method, we apply it first to the case in which the phase shifts are obtained from a given model potential. No existence problem arises in this case even if the data set is overdetermined. As the model potential we choose the Woods-Saxon (WS) potential

$$V_{WS}(r)=\frac{W_0}{1+\exp[(r-r_w)/a_w]} .$$

For the functions $\{\varphi_i\}$ we employ the standard oscillator basis

$$\varphi_i(r)=N_{i-1}\exp\left[-\tfrac{1}{2}\left[\frac{r}{r_0}\right]^2\right]L_{i-1}^{\frac{1}{2}}\left[\left[\frac{r}{r_0}\right]^2\right]$$

with various values of the parameter r_0 (here L_n^m are the generalized Laguerre polynomials).

The starting approximation to the potential must be chosen so as to describe the phase shifts qualitatively and to ensure the necessary number of bound states. If the starting potential is not selected properly, no minimization procedure can yield the required minimum of χ^2. It is not easy to give a general prescription for the starting potential and any information about the true potential may be useful. For instance, estimates of the volume integral of the true potential are sometimes available. All our numerous calculations confirm that the Gaussian potential selected so that its volume integral is equal to that of the exact potential constitutes a very good starting approximation, i.e., we choose $V^{(0)}(r)$ as

$$V^{(0)}(r)=c_1^{(0)}\varphi_1(r),\quad \varphi_1(r)=N_o\exp\left[-\frac{1}{2}\left[\frac{r}{r_0}\right]^2\right],$$
$$c_1^{(0)}=\frac{\int V_{\mathrm{WS}}(r)r\,dr}{\int \varphi_1(r)r\,dr} . \qquad (13)$$

In our calculations we used input data of various forms (see Table I). The quality of the solution of the inverse problem, i.e., the accuracy with which the phase shifts are reproduced, is given by the value of χ^2 and by the deviation of the reconstructed potential from the true one defined as

$$\varepsilon_v=\int[V_{\mathrm{WS}}(r)-V(c_i,r)]^2dr . \qquad (14)$$

Besides these quantities, Table I also shows the expansion coefficients c_i. In the majority of cases we used the oscillator basis with $N=9$. The blank spaces in the table indicate the cases in which a basis of lower dimension was used. In some cases enlargement of the basis did not lead to convergence of the algorithm. This is indicated in the table as "nonconverged," and the occurrence of nonconvergence means that the information contained in the input phase shifts is not sufficient to determine the required number of coefficients. The reconstructed potentials give extremely accurate phase shifts, coinciding to four to six significant figures with the input ones (see the value of χ^2 in Table I). From these model calculations the following conclusions can be drawn.

A. Dependence of the convergence on the basis

In most cases the inversion method converges rapidly, after 3–5 iterations. When one more basis function is

TABLE I. Test of the proposed algorithm for calculation of the local potential in the form of Eq. (1) from the phase shifts generated by the Woods-Saxon potential with the parameters $W_0=-50$ MeV, $r_w=2$ fm, and $a_w=0.5$ fm. The first four columns describe the data sets used for the construction of the potential. The χ^2 values obtained from various sets of input data are in column 5. The quantity ε_v, Eq. (14), measures the deviation of the reconstructed potential from the true one. c_1-c_9 are the expansion coefficients, Eq. (1), of our potential.

	Input data sets					Reconstructed Fourier coefficients of the potential								
Case No.	l	Energy interval MeV	Number of points	χ^2	ε_v	c_1	c_2	c_3	c_4	c_5	c_6	c_7	c_8	c_9
1	0	0.1−50	11	10^{-5}	123	−62.07	11.5	0.09	0.78			nonconverged		
2	0	0.1−250	15	10^{-5}	3.6	−65.53	−26.24	−1.03	0.88	−1.05	−0.234	−0.22	−0.01	nonconverged
3	0	0.1−1500	24	10^{-4}	0.49	−65.16	−24.20	−0.707	0.933	−0.852	−0.163	−0.15	0.031	0.021
4	1	0.1−50	11	5×10^{-7}	5075	−72.3	14.5	−12.9	−11.8	−12.8	−6.32	−1.87		
5	1	0.1−100	13	3×10^{-8}	1298	−67.56	20.66	−5.35	−3.52	−5.85	−4.94	−3.97	−1.96	−0.54
6	1	0.1−150	14	2×10^{-5}	13.5	−64.94	23.91	−1.69	0.54	−1.42	−0.58	−0.65	−0.33	−0.17
7	1	0.1−180	15	10^{-5}	0.3	−64.711	24.19	−1.384	0.87	−1.06	−0.18	−0.25	−0.033	−0.06
8	1	0.1−250	15	10^{-5}	0.06	−64.690	24.212	−1.3553	0.900 03	−1.0296	−0.148	−0.22	−0.005	−0.05
9	1	0.1−1000	22	2×10^{-4}	0.004	−64.675	24.231	−1.3334	0.921 96	−1.0077	−0.125 68	−0.191 03	0.0300	0.004
10	2	0.1−50	11	10^{-5}	41 760	−118.5	−28.8	−41.6	−20.0	−6.5		nonconverged		
11	2	0.1−250	15	5×10^{-3}	0.55	−64.600	24.315	−1.23	1.01	−1.03				
12	0,1	0.1−250	18	5×10^{-5}	0.008	−64.675	24.229	−1.34	0.932	−0.98	−0.15	−0.2	0.08	2.10
13	0,1,2	0.1−50	33	2×10^{-5}	0.1	−64.675	24.230	−1.35	0.96	−0.81	−0.13	−0.15	−0.16	−0.15
14	0,1,2	0.1−250	45	4×10^{-4}	0.0035	−64.675	24.230	−1.336	0.923	−1.00	−0.132	−0.193	0.05	−0.01
15	0−4	30	5	10^{-12}	2.7	−64.702	24.329	−1.4747	0.08	−1.687				
16	0−4	50	5	5×10^{-8}	0.13	−64.688	24.241	−1.3395	0.9068	−1.0084				
17	0−4	100	15	10^{-9}	0.09	−64.602	24.175	−1.4128	−1.1542	−1.2522				
18	0−14	100	15	0.005	0.09	−64.680	24.229	−1.3381	0.916 31	−1.0648				
19	0−14	180	15	4×10^{-5}	0.003	−64.676	24.231	−1.3348	0.921 83	−1.0100	−0.124 75	−0.195 17	0.035	−0.003
20	0−14	500	15	2×10^{-6}	0.036	−64.728	24.328	−1.487	1.100	−1.065	−0.3475	−0.28	−0.44	0.25
Fourier coefficients of the test potential				0.003[a]	0.003[a]	−64.676	24.230	−1.3343	0.920 94	−1.0088	−1.127 18	−0.192 70	0.029	0.0038

[a] These entries were obtained by truncating the Fourier expansion of the test potential at $N=9$.

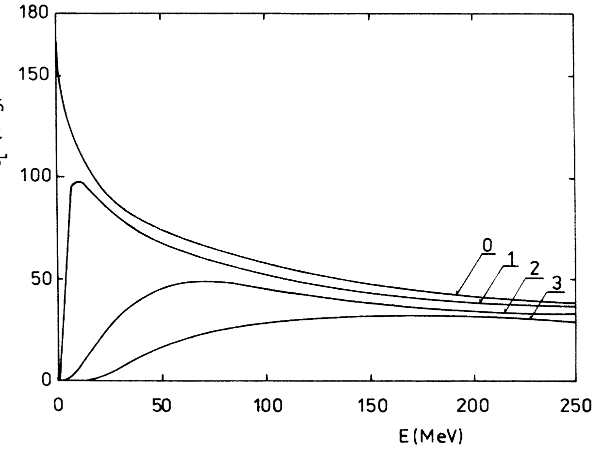

FIG. 1 Phase shifts for the Wood-Saxon potential V_{WS}.

added, convergence is usually reached after 1–2 iterations because the previous value of χ^2 was already sufficiently small. The algorithm does not converge when the basis is not properly chosen. In the case of the oscillator basis this means that a poor choice of r_0 has been made. For example, if we set $r_0=0.5$ fm, the series (1) converges so slowly that its first N terms cannot be used to reconstruct the potential V. If the input information allows for the reconstruction of the potential and the basis has not been properly chosen, the algorithm either diverges or leads to a highly oscillating solution with a large value of χ^2. When r_0 exceeds the value 1.4 fm, the convergence again becomes worse. The reconstructed potential has large oscillating tails in this case, and a large number of basis functions is necessary to get rid of them.

When the input information is not sufficient for reconstruction of the potential, the algorithm converges for a small number of basis functions, but with an increase in the number of basis functions the convergence

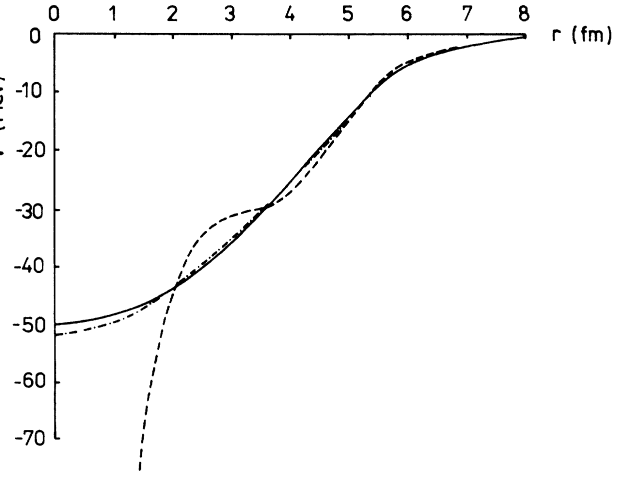

FIG. 2. Comparison of the test Wood-Saxon potential (solid line) with the reconstructed potentials: —·—·—, reconstructed from five phase shifts ($l=0$, 1, . . . ,4) at $E=30$ MeV, $\chi^2=2\times10^{-12}$; — — —, reconstructed from nine values of D phase shifts ($0.1 < E < 250$ MeV), $\chi^2=2\times10^{-18}$.

TABLE II. Convergence of the reconstructed potential at increasing number of basis functions $\varphi_N(r)$ for $N=1,2,\ldots,14$. Parameters of the Woods-Saxon potential are the same as in Table I: $E=180$ MeV, $r_0=1.1$ fm, $l=0,1,\ldots,15$. All quantities here have the same meaning as in Table I. The first line of this table corresponds to the starting approximation giving the correct value of the exact volume integral.

N	Number of iterations	χ^2	ε_v	c_1	c_2	c_3	c_4	c_5	c_6	c_7	c_8	c_9	c_{10}	c_{11}	c_{12}	c_{13}	c_{14}
1	0	443	1780	−76.37													
1	3	307	974	−66.67													
2	2	1.49	3.58	−65.48	24.574												
3	2	0.44	0.37	−64.789	24.572	−1.8082											
4	1	0.26	1.03	−64.781	24.229	−1.8177	0.848 26										
5	1	0.01	0.043	−64.683	24.219	−1.3556	0.879 71	−1.1028									
6	1	0.0065	0.016	−64.684	24.233	−1.3577	0.935 98	−1.0968	−1.3202								
7	1	2×10^{-4}	0.003	−64.676	24.232	−1.3353	0.925 91	−1.0140	−1.0943	−0.189 96							
8	1	4×10^{-5}	0.003	−64.676	24.231	−1.3350	0.921 92	−1.0103	−1.2429	−0.196 44	0.035						
9	1	4×10^{-5}	0.003	−64.676	24.231	−1.3348	0.921 83	−1.0100	−1.2475	−0.195 17	0.035	−0.0033					
10	1	2×10^{-7}	0.005	−64.676	24.230	−1.3344	0.921 05	−1.0091	−1.2665	−0.192 71	0.029	0.0005	0.025				
11	1	2×10^{-7}	0.005	−64.676	24.230	−1.3344	0.921 04	−1.0091	−1.2666	−0.192 68	0.029	0.0005	0.025	−0.0002			
12	1	2×10^{-9}	0.009	−64.676	24.230	−1.3343	0.921 00	−1.0089	−1.2706	−0.192 87	0.029	0.0036	0.032	0.009	0.008		
13	1	2×10^{-10}	0.007	−64.676	24.230	−1.3343	0.920 95	−1.0089	−1.2705	−0.192 64	0.029	0.0031	0.030	0.005	0.005	−0.002	
14	1	2×10^{-12}	0.007	−64.676	24.230	−1.3343	0.920 97	−1.0088	−1.2715	−0.192 68	0.029	0.0040	0.034	0.012	0.013	0.004	0.003
Fourier coefficients of the true potential				−64.676	24.230	−1.3343	0.920 94	−1.0038	−1.2718	−0.192 70	0.029	0.0038	0.032	0.008	0.007	−0.003	−0.004

deteriorates (see cases 1 and 10 in Table I). This serves as a confirmation of the standard fitting procedure widely used in optical-model calculations.

B. Uniqueness of the reconstructed potential

If the input phase shifts do not contain enough information to reconstruct the potential, it is possible to obtain extremely accurate phase shifts (5–7 figures coinciding), but the reconstructed potential can differ substantially from the true one (see cases 1, 4, 5, 10, and 15 in Table I). The value of χ^2 is very small (10^{-7} or even less) but ε_v is large and the reconstructed potential has nothing in common with the true one.

What information is needed for a unique reconstruction (in the sense discussed previously) of the potential? The potential under consideration possesses one bound state in the s wave and a rather narrow resonance in the p wave (see Fig. 1). Our experience shows that to reconstruct the potential from one partial wave, it is better to employ the p wave rather than the s wave, which requires phase shifts for very large energies (1–2 GeV; see cases 1–3 and 4–9 in Table I).

When the reconstruction is to be carried out at a fixed energy, one must know the phase shift for all values of l for which the phase shifts are not small, i.e., up to the region where the Born approximation becomes accurate. For example, it is sufficient to take five partial waves to calculate five expansion coefficients c_i at energy 50 MeV. The phase shifts with higher l do not carry any additional information because they are very small and the accuracy of their determination is low. The first five phase shifts permit a reasonable reconstruction of the potential even at energies as low as 30 MeV (see case 15 in Table I and Fig. 2). Of course, the central part of the potential is not well reproduced. For a further improvement of the potential, it is necessary to increase the number of phase shifts and simultaneously to increase also the energy because at $l \sim 10$–14 the phase shifts are not yet close to the Born approximation. At the energy 2 GeV the first 15 phase shifts all show little difference and do not allow a reconstruction of the potential at all. The algorithm either diverges or converges to a very large value of χ^2. Hence, to reconstruct N expansion terms of the potential at a fixed energy it is necessary to choose the energy in such a way that at $l \sim N$ the phase shifts are accurately given by the Born approximation. Addition of phase shifts at lower energies to this data set does not improve the quality of the reconstruction.

C. Relation to the Fourier analysis

There exists a close relation between the Fourier analysis and the inverse-scattering problem that allows us to use many important results, such as spectral theorems, error analysis, etc. Namely, the phase shifts are given by Eq. (10) as

$$\tan\delta_k = X_k = \int V(r) Y_k(r)\,dr \ , \tag{15}$$

where

$$Y_k(r) = -\frac{1}{p}\frac{2m}{\hbar^2} F_{lk}(p_k r)\psi_{lk}(p_k, r) \ . \tag{16}$$

This means that we are given a set of "Fourier coefficients" X_k of the unknown potential V with respect to a system of unknown nonorthogonal functions $Y_k(r)$. These functions are not normalizable, but this causes no difficulty because the potential is assumed to be short ranged. Moreover, Hylleraas[10] proved that the functions $Y_k(r)$ generate a biorthogonal basis and found the corresponding biorthogonal complement. In all real cases it is assumed that the potential is confined to a finite range and attains its asymptotic form at some distance R. The inverse-scattering problem can now be formulated as the problem of finding N Fourier coefficients $\{c_i\}$ with respect to the basis $\{\varphi_i\}$, given M coefficients $\{X_k\}$ with respect to the unknown basis $\{Y_k\}$. To do so the set of functions $\{Y_k\}$ must be complete in the space spanned by the functions $\{\varphi_i\}$. For example, if $\{\varphi_i\}$ is a polynomial basis, then φ_N has N zeros. Hence, the input data set must allow the construction of an N-zero function from the functions Y_k. To reconstruct the potential from one partial-wave phase shift, energies up to $pR \sim N\pi$ (R is the interaction radius) are needed.

Evidently, from a finite number of input data we can determine only a finite number of the expansion coefficients c_i, and their accuracy decreases with increasing i. This behavior is demonstrated by the examples collected in Table II. This situation is analogous to the Fourier analysis of a signal containing noise passing through a filter with a finite bandwidth. We recall that the complete system of orthonormal functions $\{\varphi_i\}$ possesses the following property: in approximating a function $f(x) \approx f^N(x) = \sum_{i=1}^{N} c_i \varphi_i$ by the least-squares method the minimum of $\chi^2 = \int [f(x) - f^N(x)]^2 dx$ is obtained by setting $c_i = \int f(x)\varphi_i(x)\,dx$, and with increasing N the previously determined coefficients c_i do not change. This property is approximately satisfied by our method of reconstructing the potential from the phase shifts (see Table II).

A few words on the errors in the coefficients c_i calculated from inexact experimental phase shifts are now in order. In our linear approximation,

$$\Delta c_i = \sum_k \left| \frac{\partial c_i}{\partial \delta_k^{\text{expt}}} \right| \Delta\delta_k^{\text{expt}} \ , \tag{17}$$

where the function $c_i(\delta_k^{\text{expt}})$ are given by Eq. (6). Hence

$$\frac{\partial c_i}{\partial \delta^{\text{expt}}} = 2 \sum_j (A^{-1})_{ij} \frac{\partial \delta_k}{\partial c_j} \ , \tag{18}$$

where A_{ij} and $\partial\delta_k / \partial c_j$ are evaluated at the minimum of χ^2. Assuming that all the phase shifts have a uniform error ϵ, i.e., $\Delta\delta_k \le \epsilon |\delta_k^{\text{expt}}|$, we obtain the estimate

$$\frac{\Delta c_i}{c_i} \le \frac{\epsilon}{c_i} \sum_k \left| \frac{\partial c_i}{\partial \delta_k^{\text{expt}}} \right| |\delta_k^{\text{expt}}| \ . \tag{19}$$

Some characteristic values of $\Delta c_i / c_i$ are given in Table III. From this table we conclude that the approximation error grows rapidly with increasing i and for $i \ge 5$ exceeds

TABLE III. Error estimates of the parameters c_i, $(\Delta c_i/c_i)(1/\epsilon)$, for a unique relative error ϵ of the input data for case 19 (see Table I).

	$(\Delta c_i/c_i)(1/\epsilon)$								
N	$i=1$	2	3	4	5	6	7	8	9
1	0.0026								
2	0.001	0.07							
3	0.026	0.025	2.4						
4	0.017	0.18	1.49	13.4					
5	0.029	0.086	3.9	6.2	13.2				
6	0.038	0.28	5.4	15.3	18.3	324			
7	0.057	0.19	7.8	12.0	12.8	287	251		
8	0.061	0.29	7.4	19.5	18.3	125	278	2000	
9	0.091	0.34	10.6	22.0	28.0	220	113	2311	33 203

TABLE IV. Parameters of the reconstructed electron-atom potentials (in atomic units).

Atom	α_p	r_p	r_0	r_B	z	c_1	c_2	c_3	c_4
Ne	2.663	0.85	0.430 14	0.430 14	10.219	−1.1365	5.5585	−7.0083	2.1652
Ar	11.08	1.5	0.5	1.0	16.67	0.890 22	0.091 46	−0.0206	0

TABLE V. Comparison of the phase shift calculated with our reconstructed potential (columns denoted by *a*) with the input phase shift (denoted by *b*) for neon and argon. The energies used for the reconstruction are in the first column; $l=0,1,\ldots,3$ is the angular momentum.

		$l=0$		$l=1$		$l=2$		$l=3$	
Atom	E (eV)	*a*	*b*	*a*	*b*	*a*	*b*	*a*	*b*
Ne	0.1361	−2.3178	−2.2918	0.1727	0.1719	0.0443	0.0458	0.0123	0.0172
	0.5442	−6.5235	−6.8755	0.2006	0.2636	0.1894	0.1833	0.0599	0.0630
	1.2245	−11.8807	−12.0894	−0.3908	−0.2349	0.4660	0.4354	0.1376	0.1375
	1.9958	−16.8657	−16.6158	−1.4304	−1.1459	0.8325	0.7448	0.2314	0.2235
	3.4015	−24.3339	−23.8923	−3.6238	−3.3232	1.6083	1.3751	0.4268	0.3896
	4.8982	−30.8626	−30.2522	−5.9982	−5.6723	2.5103	2.1658	0.6733	0.5730
	6.6669	−37.3435	−36.6693	−8.6676	−8.4798	3.5853	3.1513	1.0071	0.8021
	8.7078	−43.6655	−42.9718	−11.4989	−11.4592	4.7698	4.0107	1.4256	1.0886
	11.0209	−49.7625	−49.2743	−14.3850	−14.3239	6.0130	5.7296	1.9120	1.4209
	13.6060	−55.6014	−56.0925	−17.2462	−17.7044	7.2949	7.2193	2.4396	1.8163
	19.5926	−66.4753	−68.1246	−22.6889	−23.4913	10.0282	10.4851	3.5248	2.7445
Ar	0.0999	2.5909	2.5497	0.6492	0.6761	0.1289	0.1375	0.0286	0.0458
	0.1361	2.2984	2.2460	0.8149	0.8480	0.1842	0.1891	0.0510	0.0632
	0.1999	1.5918	1.5642	1.0566	1.1001	0.2736	0.2750	0.0868	0.0917
	0.3004	0.2842	0.2865	1.3219	1.3980	0.4215	0.4240	0.1321	0.1375
	0.4002	−1.0776	−1.0829	1.4753	1.5642	0.5735	0.5787	0.1789	0.1833
	0.5442	−3.0495	−2.9679	1.5604	1.6673	0.7998	0.8079	0.2467	0.2521
	1.2245	−11.5350	−11.1727	0.6774	0.7391	2.0727	2.0455	0.5644	0.5730
	2.0000	−19.6065	−19.0050	−1.4720	−1.6215	3.9359	3.8331	0.9625	0.9568
	3.0005	−28.2643	−27.6280	−4.7628	−5.3170	6.8990	6.7953	1.5607	1.4782
	3.4015	−31.3262	−30.7220	−6.1183	−6.8640	8.2330	8.2048	1.8284	1.7017
	3.9999	−35.5544	−35.0822	−8.1224	−9.1730	10.3565	10.5138	2.2537	2.0397
	4.9999	−41.8782	−41.6998	−11.3608	−12.9546	14.2211	14.9370	3.0223	2.6299
	6.0006	−47.4750	−47.6414	−14.4217	−16.5871	18.4475	19.9962	3.8443	3.2601
	7.0005	−52.4953	−53.0616	−17.2929	−20.0421	23.0091	25.5711	4.6984	3.9190
	8.0001	−57.0533	−58.0348	−19.9832	−23.3079	27.8967	31.5241	5.5704	4.6008
	8.9998	−61.2327	−62.6414	−22.5101	−26.4076	33.0988	37.6777	6.4490	5.2999
	9.9999	−65.0952	−66.9271	−24.8875	−29.3240	38.5891	43.8599	7.3279	6.0103
	15.0006	−80.9765	−84.7290	−34.9958	−41.8259	67.9162	70.5368	11.5800	9.6142

10ϵ. This means that if the experimental error is, say, 10%, we cannot determine more than five expansion coefficients.

IV. ELECTRON-ATOM SCATTERING

The interaction between an electron and an atom is very complicated. Exchange of the incident electron with the atomic electrons is an important effect at low and intermediate energies. In the Hartree-Fock theory the exchange potential is nonlocal, and this fact considerably complicates the calculations. A phase-shift equivalent local exchange potential offers practical advantages from a computational point of view and can also afford insight into the exchange effect.[8] Consequently a number of approximate local exchange potentials have been proposed.[11-14] These potentials are given analytically and are simple to apply. The effective interaction consists of three terms

$$V=V_s+V_{\rm ex}+V_p \; , \tag{20}$$

where V_s is the static interaction, $V_{\rm ex}$ is the local exchange potential, and V_p is the polarization interaction which accounts for virtual excitations of the atom. As an example of localization of the exchange interaction we quote the so-called $X\alpha$ approximation used recently[15,16] to calculate elastic scattering of electrons on Ar and Ne. In this approximation the local exchange potential reads

$$V_{\rm ex}(r)=-\tfrac{3}{2}\alpha\left[\frac{3}{\pi}\right]^{1/3}\rho^{1/3}(r)\; . \tag{21}$$

Here, $\rho(r)$ denotes the total charge density and α is a free parameter. The $\rho^{1/3}$ dependence has been introduced by Slater[17] and has been widely used in many areas. In contrast to the approaches in which an analytic form of the exchange potential is assumed, the proposed inverse scattering method allows us to find local effective potentials without any *a priori* assumptions about the shape of such potentials.

We represent the local effective potential as follows:

$$V(r)=V_p(r)-\frac{2Z}{R}e^{-r/r_0}-2e^{-r/r_B}\sum_{i=1}^{N}c_i r^{i-1} \tag{22}$$

with

$$V_p(r)=-\alpha_p\frac{1-e^{-r/r_p}}{(r^2+r_p^2)^2}\; , \tag{23}$$

where α_p is the experimentally determined polarizability of the atom.[18] As the input data we use the phase shifts calculated in Ref. 19 for $l=0$, 1, 2, and 3 for Ne and Ar. Our algorithm makes it possible to find not only the linear expansion coefficients c_i and Z but also the nonlinear parameters r_0 and r_B. The algorithm is not always convergent with respect to the nonlinear parameters, but when the iterations do converge they usually converge very rapidly.

Parameters of the reconstructed potentials are collected in Table IV, and the calculated phase shifts are compared with the input ones in Table V. Figure 3 shows a comparison of our potential obtained for Ne and Ar atoms from the phase shifts calculated by Nakanishi and Schrader[19] with the well-known Herman-Skillman potential[20] (dots) and with the $X\alpha$ approximation (circles). In the latter case we set $\alpha=0.55$, which is the commonly accepted value.[15] In Fig. 3 only the short-range part of the respective potentials is plotted; the polarization part, which is identical in all three cases, has been omitted. Both the Herman-Skillman potential and the $X\alpha$ approximation potential are typical atomic structure potentials defined in terms of charge density. Although our potentials result from pure scattering data, they are very close to the Herman-Skillman and $X\alpha$ potentials in a very broad region. It should be noted, however, that in spite of their similarity, their phase shifts differ substantially from each other. These results indicate that the low-energy electron–noble-gas-atom phase shifts calculated with a complicated energy-dependent exchange potential[19] can be well described in terms of a simple local static potential. We have applied our potentials to the calculation of the induced bremsstrahlung cross sections of electrons on atoms in laser field for which the off-energy-shell scattering amplitude is needed.[21]

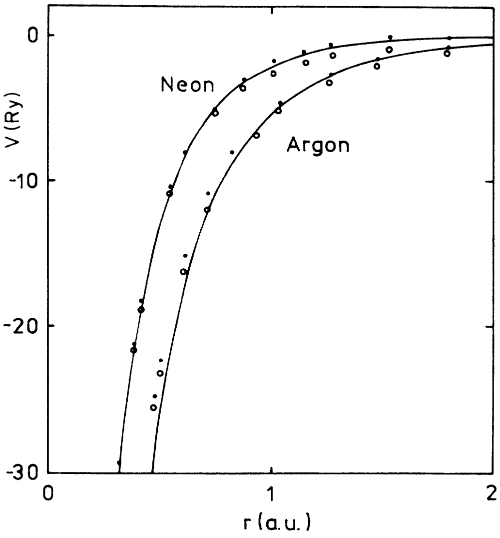

FIG. 3. Comparison of the reconstructed potentials (solid line) with the Herman-Skillmann potential (dots) and the X_α approximation (circles) for $e^- +$ Ne and $e^- +$ Ar low-energy scattering.

V. CONCLUSION

In this paper an efficient method for calculation of the potential from a (finite) set of phase shifts has been proposed. The principal features of the method are as follows. The inversion gives a local energy-independent potential, whose form is not assumed in advance. The method is iterative, very fast, and uses all the data simultaneously, i.e., it makes use of the knowledge of the phase shifts at various energies and various momenta in a single analysis. The method has been tested in detail for model potentials, its convergence has been studied, and a relation to Fourier analysis has been discussed. The method has proved to be very efficient. The present paper has been aimed at studying the general properties of the inversion method. A subsequent paper is planned to be devoted to the inversion of realistic data.

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[1] I. M. Gelfand and B. M. Levitan, Dokl. Akad. Nauk SSSR **77**, 555 (1951).

[2] V. A. Marchenko, Dokl. Akad. Nauk SSSR **104**, 695 (1955).

[3] R. G. Newton, J. Math. Phys. **3**, 75 (1962).

[4] A. A. Ioannides and R. S. Mackintosh, Nucl. Phys. A **438**, 354 (1985).

[5] R. Lipperheide *et al.*, Phys. Rev. C **26**, 770 (1982).

[6] M. Coz, H. V. von Geramb, and J. D. Lumpe, Z. Phys. A **328**, 259 (1987); J. Kuberczyk, M. Coz, H. V. von Geramb and J. D. Lumpe, *ibid.* **328**, 265 (1987).

[7] K. E. May, M. Münchov, and W. Scheid, Phys. Lett. B **141**, 1 (1984).

[8] G. Staszewska, J. Phys. B **22**, 913 (1989).

[9] P. R. Bevington, *Data Reduction and Error Analysis for the Physical Sciences* (McGraw-Hill, New York, 1969), p. 232.

[10] E. A. Hylleraas, Phys. Rev. **74**, 48 (1948).

[11] E. W. Holler and L. J. Allen, Phys. Rev. A **33**, 3774 (1986).

[12] B. H. Brandsden, M. R. C. Dowel, C. J. Noble and T. Scott, J. Phys. B **9**, 1301 (1976).

[13] J. B. Furness and I. E. McCarthy, J. Phys. B **6**, 2280 (1973).

[14] M. E. Riley and D. G. Truhlar, J. Chem. Phys. **63**, 2182 (1975).

[15] H. P. Berg, Physica B+C **122**, 129 (1983).

[16] H. Gollisch, J. Noffke, and F. Pasemann, Physica B+C **128**, 91 (1985).

[17] J. C. Slater, Phys. Rev. **81**, 385 (1951).

[18] E. J. Robinson and S. Geltman, Phys. Rev. **153**, 4 (1967).

[19] H. Nakanishi and D. M. Schrader, Phys. Rev. A **34**, 1823 (1986).

[20] F. Herman and S. Skillman, *Atomic Structure Calculations* (Prentice-Hall, Englewood Cliffs, NJ, 1963).

[21] V. N. Pomerantsev *et al.*, Fiz. Plazmy **15**, 326 (1989).