Wesley, Cambridge, Mass., 1955), 1st ed., Sec. 11.2. ⁸K. Marko, private communication.

⁹K. I. Roulston and S. I. H. Naqvi, Nucleonics Data Sheet 21, 1964.

¹⁰See, for example, R. Hagedorn, *Relativistic Kine-matics* (Benjamin, New York, 1964), 1st ed., Chap. 7.

¹¹A more detailed calculation of this branching ratio

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(1953).

to the noise is negligible.

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Numerical Computations in the Inverse-Scattering Problem at Fixed Energy

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Constructing potentials from the phase shifts at a given energy yields an infinity of equivalent solutions. The deviations of these solutions from each other can, however, be analyzed according to *a priori* limitations on the derivatives and other features of "acceptable" potentials. A sketch of this analysis is given together with a numerical comparison of usual potential forms with the equivalent potentials obtained through Newton's method. The observed deviation gives an appraisal of the deviations from each other of all the equivalent potentials with similar bounds on the derivatives. The deviation is small when there are many phase shifts available, all of them definitely smaller than $\pi/2$. For a static potential these conditions can be met for high energies.

We study the elastic scattering of a particle obeying the Schrödinger equation with a spherically symmetric potential, at an energy $E = \hbar^2 k^2/2m$, m being the reduced mass and k being the linear momentum. The "inverse problem" deals with the construction of the potential from the phase shifts. We therefore assume that the phase shifts have already been derived from the cross section - not a trivial assumption.¹ Once the phase shifts are known, many theoretical papers give us formal ways of obtaining the potential.

The seemingly simplest method is to use the JWKB formula for the phase shift, which yields δ_i as a Riemann-Liouville transform of a function associated with the potential and therefore reduces this step of the inverse problem to solving an Abel integral equation. This situation has been encountered a long time ago in other inverse problems, going from the Wiechert-Herglotz-Bateman method in seismology² to well-known results in spectrometric measurements.³ In quantum mechanics it has been used by several authors.⁴ However, some steps of the method are questionable as regards the problem studied in the present paper. Actually, the interest of such a method does not really reside in solving the inverse problem, but in reducing the computing time for obtaining a potential which fits the phase shifts; it does not give any information on how far from this potential may be

other potentials fitting the same set of phase shifts. In short, it extracts from the phase shifts very much biased information. So does the computer⁵ when, working by trial and error, it fits the phase shifts by matching three parameters in a Woods-Saxon potential.

has been made by McCoyd [G. C. McCoyd, Ph.D. thesis,

result was $R(^{1}S \rightarrow 4\gamma)/R(^{1}S \rightarrow 2\gamma) \approx 3 \times 10^{-7}$ as compared to our estimate of 2×10^{-8} . In either case this contribution

¹²F. G. Fumi and L. Wolfenstein, Phys. Rev. 90, 498

St. Johns University, N. Y., 1965 (unpublished)]. His

However, the main interest of solving the inverse problem by inverse methods (viz., by methods which are not trial and error ones), is to obtain an evaluation of the amount of information contained in the scattering amplitude. Now we know, from the formal methods of Regge, ⁶ Newton, ⁷ Sabatier, ⁸ and Loeffel, ⁹ that an infinity of potentials corresponds to a given set of phase shifts. The "Regge-Loeffel" methods⁹ are not suitable for computation, nor is the Martin-Targonski method, ¹⁰ which is of physical interest because it deals with generalized Yukawa potentials.

On the other hand, the so-called¹¹ Newton-Sabatier methods are easy to handle on a computer, but one has first to answer the following fundamental question: Let us take for granted that the "physical properties" of the potential can be mathematically expressed through bounds on the derivatives. Then, if a potential is constructed from its phase shifts by one of the above methods, how different can the result be from the original potential?

There are two complementary ways of answering this question. The first is to define for the problem a mathematical frame, set a convenient metric on the space of acceptable potentials, study the continuity of the various steps involved in an inverse method, and finally enclose all the possible mappings of a set of phase-shifts into the class of potentials in a closed set whose diameter is to be evaluated when different physical parameters (including energy) afford additional constraints. This is the object of a forthcoming paper by one of the authors.^{12, 13}

The second way is to use the partial information already available on the reliability of the simplest of the above methods and to check it on a computer under the conditions which have proved to be of interest in the mathematical analysis. This study is the object of the present paper.

We use the simplest of the quoted methods, ⁷ the one in which the "input function" f(r, r') is expanded in the physical wave functions

$$f(r,r') = \sum_{0}^{\infty} c_{1}u_{1}(r)u_{1}(r'), \qquad (1)$$

where the coefficients c_i are bounded. Let $A_i \sin(r - \frac{1}{2}l\pi + \delta_i)$ be the asymptotic behavior of the regular wave functions. We know⁷ that the coefficient c_i can be obtained from the phase shifts by solving the equation

$$\tan \delta_{l} = \sum_{l'} \mathcal{M}_{l}^{l'} a_{l'} (1 + \tan \delta_{l} \tan \delta_{l'}), \qquad (2)$$

where $M_l^{l'}$ is equal to $[(l' + \frac{1}{2})^2 - (l + \frac{1}{2})^2]^{-1}$ for odd (l - l') and 0 for even (l - l'), and substituting the values of a_l in the formulas

$$b_{l} = a_{l} (\cos \delta_{l})^{-1},$$
(3)

$$A_{l} = \cos \delta_{l} - \frac{1}{2} \pi b_{l} / (2l+1) - \sum M_{l}^{l'} b_{l'} \sin(\delta_{l'} - \delta_{l}),$$

$$c_{t} = b_{t}(A_{t})^{-1}.$$
(4)
(5)

Using matrix notations, 7 we write the solution of (2) in the form

$$\mathbf{\tilde{a}} = (1+R)^{-1} (\alpha \mathbf{\tilde{\nabla}} + M^{-1} \tan \Delta \mathbf{\tilde{e}}), \tag{6}$$

where

$$R = M^{-1} \tan \Delta M \tan \Delta, \tag{7}$$

$$M^{-1} = -\mu M \mu, \qquad (8)$$

$$v_{2l} = \mu_{2l} = \frac{2}{\pi} (4l+1) \left[\frac{\Gamma(l+\frac{1}{2})}{\Gamma(l+1)} \right]^2,$$
(9)

$$\mu_{2l+1} = \frac{2}{\pi} (4l+3) \left[\frac{\Gamma(l+\frac{3}{2})}{\Gamma(l+1)} \right]^2, \tag{10}$$

$$v_{2l+1} = 0,$$
 (11)

and \bar{e} is the unit vector. The specification of the method, called \mathfrak{M}_{0} in the following, is achieved by

choosing α in such a way that the potential decreases faster than $r^{-3/2-\epsilon}$ for large r. α is therefore given from the phase shifts by a secondary calculation?⁷ In the following we call this the α specification. Formulas (6), (3), (4), and (5) therefore yield the c_1 's from the δ_1 's. The potential is then obtained from f(r, r') through the integral equation

$$K(r,r') = f(r,r') - \int_0^r K(r,\rho) f(\rho,r') \rho^{-2} d\rho \qquad (12)$$

and the formula

$$V(r) = -2r^{-1}\frac{d}{dr}[r^{-1}K(r,r)].$$
 (13)

Let us now sketch the available information obtained from the mathematical analysis of this method. For very weak assumptions on the δ_l asymptotic behavior, ⁷ it is known that the c_l 's, thanks to the " α specification," go to a constant as l goes to infinity, plus $O(l^{-2})$. Now it has been shown by Sabatier^{12,13} that f(r, r') can then be written as follows:

$$f(r, r') = f_0(r, r') = 2rr' \int_0^1 \frac{\sin kw}{w} F(k, t) t dt, \quad (14)$$

where

$$w = [(r - r')^2 + 4rr't^2]^{1/2}, \qquad (15)$$

$$F(k, t) = \gamma t^{-1} + F_1(k, t);$$
(16)

 γ is equal to the potential moment $\int_0^{\infty} \rho V(\rho) d\rho$, times a numerical constant. $F_1(k, t)$ is a function of t, integrable on [0, 1]. Now it can be shown¹³ that, for any potential of a very large class $\overline{\mathcal{S}}$, including for instance the potentials whose secondorder derivative does not diverge more rapidly than r^{-3} at the origin, and goes to zero faster than r^{-5} as r goes to ∞ , the function f(r, r') can be put in the form

$$f(\mathbf{r},\mathbf{r}') = 2\mathbf{r}\mathbf{r}' \int_0^\infty \frac{\sin kw}{w} F(k,t) t dt, \qquad (17)$$

where F(k, t) is given by (16), $F_1(k, t)$ being integrable from 0 to ∞ . The comparison of $f_0(r, r)$ and f(r, r) is interesting. Let us introduce the function

$$S_1(u, k) = k^{-1}F_1(k, u/k)$$
 (18)

and a function S(u, k) equal to $S_1(u, k) + \gamma u^{-1}$. It is easy to see that

$$r^{-1}f_0(r,r) = \int_0^R \sin(2ur)S(u,k)du,$$
 (19)

whereas f(r, r) is given by

$$r^{-1}f(r,r) = \int_0^\infty \sin(2ur) S(u,k) du.$$
 (20)

In addition, it can be shown¹² that, for any static

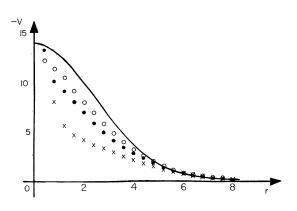


FIG. 1. Reliability as a function of energy. $V_I = -14 e^{-(r/3.5)^2}$ (solid line). E = 10 MeV (crosses), 50 MeV (dots), 150 MeV (open circles).

potential in $\overline{\mathcal{E}}$, S(u, k) is uniformly bounded by u^{-1} times a function of k decreasing faster than k^{-1} as k goes to infinity. We refer to this as the damping effect of the energy. With these results it is easy to characterize the method \mathfrak{M}_{0} .

First, let us notice that since f(r, r') necessarily has the form (14), and since its general form for a potential of $\overline{\mathcal{E}}$ is (17), \mathfrak{M}_0 is characterized by a truncation of the Fourier spectrum of f(r, r). One can say in an equivalent way, from a glance at Eq. (19), that as regards the function [r - f(r, r)], the scattering experiment is a linear filter of width k. Now, except in the first-order approximation, f(r,r) is not K(r,r), which would readily yield the potential through (13). But there is a one-to-one correspondence between f(r, r) and K(r, r), so that one has the feeling that a close approximation to f(r,r) yields a close approximation to K(r,r). This can be proved, ¹³ provided there is no trouble in the inversion of (1+R) and of (12), viz., essentially, provided one is far from any resonance. We are then led to analyze the features of the approxima-

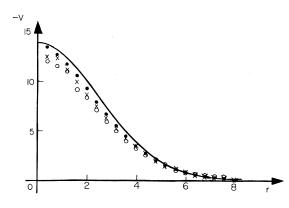


FIG. 2. Reliability as a function of energy. V_I = $-14 e^{-(r/3.5)^2}$ (solid line). E = 200 MeV (open circles), 400 MeV (crosses), 1200 MeV (dots).

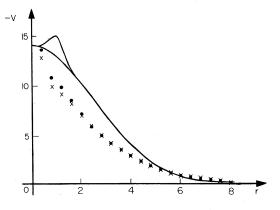


FIG. 3. Reliability for a perturbation in a central position. $V_I = -14 e^{-(r/3.5)^2} - 2e^{-[(r-1)/0.4]^2}$ (solid line); E = 50 MeV. Crosses – unperturbed Gaussian; dots – Gaussian with perturbation.

tion of f(r, r) by $f_0(r, r)$. They readily follow from (19) and from the damping effect. Comparing (19) and (20), we see that if all the derivatives of f(r, r)are bounded by numbers smaller than k, the even ones being zero, f(r, r) reduces to $f_0(r, r)$. Since bounds for the derivatives of f(r, r) can be more or less easily related, through (12), to equivalent quantities for K(r, r), it can be seen that the potentials of $\overline{\mathcal{E}}$ yielding the same set of phase shifts are generally closer to the potential yielded by \mathfrak{M}_0 , as their derivatives are bounded by smaller numbers. Moreover, the deviation of these potentials from each other should become smaller as k gets larger not only because of the increase of the filter bandpass, but also because of the energy-damping effect, which simultaneously makes the linear approximation more valid. Thus, roughly speaking, every result true for f(r, r) will be increasingly true for K(r, r). Now taking into account the fact that in a real problem only a limited number of

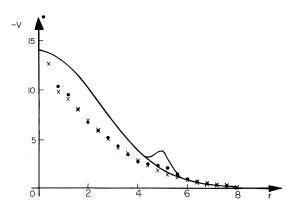


FIG. 4. Reliability for a perturbation in a surface position. $V_I = -14 e^{-(r/3.5)^2} - 2e^{-[(r-5)/0.4]^2}$ (solid line); E = 50 MeV. Crosses – unperturbed Gaussian; dots – Gaussian with perturbation.

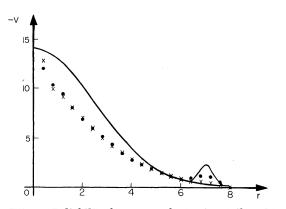


FIG. 5. Reliability for a perturbation in a tail position. $V_I = -14 e^{-(r/3.5)^2} - 2e^{-[(r-7)/0.4]^2}$ (solid line); E = 50 MeV. Crosses – unperturbed Gaussian; dots – Gaussian with perturbation.

phase shifts are known, we can determine the features of the method \mathfrak{M}_{0} :

(1) Out of the infinity of equivalent potentials in the set $\overline{\mathscr{E}}$, which certainly contains all the physically interesting potentials, \mathfrak{M}_0 selects the one for which the sine Fourier spectrum of a function f(r, r), having a one-to-one correspondence with V(r), is restricted to the interval (0, k).

(2) If all the phase shifts are bounded away from $\pi/2$, the properties of f(r, r) and K(r, r) are somewhat similar. For large energies, the damping effect makes the linear approximation f(r, r) = K(r, r) even more valid. Therefore, especially at those energies, the "distance" between equivalent potentials can be characterized by the "distance" between the corresponding functions f(r, r).

(3) If, in the infinite set of equivalent potentials in $\overline{\mathcal{S}}$, physical constraints, by absolutely bounding the derivatives of V(r), select a subset, this subset either contains \mathfrak{M}_0 or else its distance to \mathfrak{M}_0 becomes smaller and smaller as F increases or as

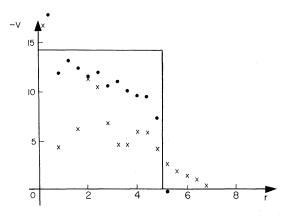


FIG. 6. Reliability as a function of potential shape: square potential of depth 14 MeV, range 5 F; E = 50 MeV (crosses), 400 MeV (dots).

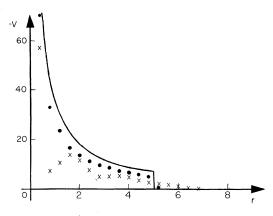


FIG. 7. Reliability as a function of potential shape: $V_I = -35/r$ for $r \le 5$, $V_I = 0$ for r > 5; E = 50 MeV (crosses), 400 MeV (dots).

the bounds on the derivatives are taken smaller.

(4) The best conditions for application of \mathfrak{M}_0 are therefore met when a large number of phase shifts smaller than or around $\pi/4$ are produced by the potential.

Now it is clear that these remarks can be put in a precise form relating the bounds of various quantities. It is clear also for any one knowing the roughness of the bounds usually derived by analytic methods that well-chosen computations can lead to an equally good feeling for the result.

NUMERICAL COMPUTATIONS

The numerical calculations¹⁴ were done on a small computer (IBM 360-40), and yet, the determination of a potential from 16 phase shifts took less than two minutes. A set of 28 phase shifts¹⁵ was computed by integrating the Schrödinger equation for various potentials and various energies listed below, chosen in such a way as to give examples of the influence of the parameters involved.

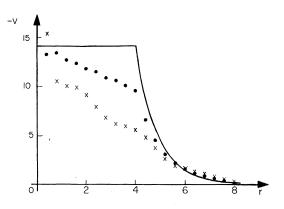


FIG. 8. Reliability as a function of potential shape: $V_I = -14$ for $r \le 4$, $V_I = -14 e^{-(4-r)/0.85}$ for r > 4; E = 50MeV (crosses), 400 MeV (dots).

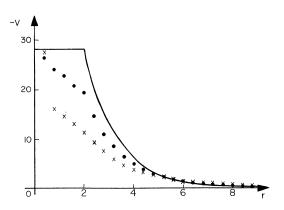


FIG. 9. Reliability as a function of potential shape: $V_I = -28$ for $r \le 2$, $V_I = -28e^{(2-r)/1.25}$ for r > 2; E = 50 MeV (crosses), 400 MeV (dots).

From every set of phase shifts, a potential is derived through \mathfrak{M}_0 . It is clear from the above analysis that the distance of this potential from the input potential gives an appraisal of the range of the set of equivalent potentials when physical constraints, such as bounds on the derivatives, are imposed on the desired potential – these constraints being exhibited in the input potential. It gives, therefore, an appraisal of what would be the reliability of any inverse method at fixed energy if the physical potential were required to fulfill these conditions.

For the sake of simplicity, typical cases of a nucleon¹⁶ in a potential are taken. The range of energy for which the method \mathfrak{M}_0 is reliable¹⁷ is in general too high to be physically interesting. However, convenient modifications of the units of length and energy may reduce physically interesting cases of colliding atoms to these cases.¹⁶ The following analyses have been undertaken, in which all the lengths are in F and all the energies in MeV. In all the figures the solid line is for the input potential, referred to as V_I , the various dotted lines for the potentials obtained through \mathfrak{M}_0 , at various en-

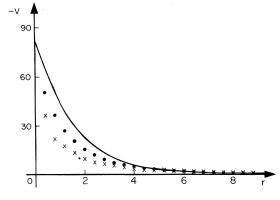


FIG. 10. Reliability as a function of potential shape: $V_I = -80e^{-r/1.50}$; E = 50 MeV (crosses), 400 MeV (dots).

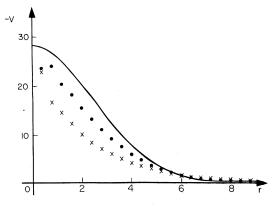


FIG. 11. Reliability as a function of potential shape: $V_I = -28e^{-(r/3.5)^2}$; E = 50 MeV (crosses), 400 MeV (dots).

ergies.

RELIABILITY AS A FUNCTION OF THE ENERGY

The potential $V = -14\exp\left[-(r/3.5)^2\right]$ generates the phase shifts. The potentials obtained through \mathfrak{M}_0 are given, for various values of the energies: 10, 50, 150, in Fig. 1 and 200, 400, 1200 in Fig. 2. The results are fairly good from 50 MeV up. They are systematically *below* the departure potential. This feature is true also for other shapes, as seen below. We do not propose any explanation. Notice that for $E \gtrsim 50$, the variations of the output potential with E are small, and not larger than the ones obtained from optical-model analyses (at different energies). This destroys arguments such as: \mathfrak{M}_0 could not be used for experimental analyses because it yields, from phase shifts generated by a static potential, an energy-dependent potential.

RELIABILITY FOR SMALL PERTURBATIONS TO THE POTENTIAL

A perturbation to the Gaussian potential has been introduced in a central position (Fig. 3), surface

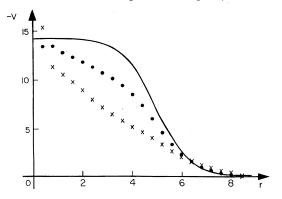


FIG. 12. Reliability as a function of potential shape: $V_I = -14[1 + e^{(r-5)/0.65}]^{-1}$; E = 50 MeV (crosses), 400 MeV (dots).

position (Fig. 4), and external position (Fig. 5) for a "bad" value of E. It is reproduced qualitatively, but not quantitatively.

RELIABILITY AS A FUNCTION OF THE SHAPE OF THE POTENTIAL

Studies have been made, for E = 50 and E = 400MeV, for square-well (Fig. 6), truncated Coulomb (Fig. 7), flat exponential (Figs. 8 and 9), exponential (Fig. 10), Gaussian (Fig. 11), and Woods-Saxon (Fig. 12) potentials. They should be compared with Figs. 1 and 2 for the Gaussian potential. Oscillations appear in the output potential whenever a de-

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¹C. E. Fröberg, Arkiv. Mat. Astron. Fysik. <u>B36</u> band 11, 50 (1949); J. H. Crichton, Nuovo Cimento <u>45</u>, 256 (1966); R. G. Newton, J. Math. Phys. <u>9</u>, 2050 (1968); A. Martin, Nuovo Cimento <u>59</u>, 131 (1969); I. A. Sakmar, Lett. Nuovo Cimento <u>2</u>, 256 (1969); R. B. Gerber and M. Karplus, Phys. Rev. D <u>1</u>, 998 (1970).

²See, for example, H. Bouasse, *Séismes et Sismo*graphes (Delagrave, Paris, 1923), p. 259, or M. Bath, *Mathematical Aspects of Seismology* (Elsevier, Amsterdam, 1968), p. 322.

³See, for example, G. Hörman, Z. Physik <u>97</u>, 539 (1935), or G. N. Minerbo and M. E. Levy, Siam. J. Numer. Anal. 6, 598 (1969).

⁴Q. B. Firsov, Zh. Eksperim. i Teor. Fiz. <u>24</u>, 279 (1953); J. A. Wheeler, Phys. Rev. <u>99</u>, 630 (1955); P. C. Sabatier, Doctorat d'état, Orsay, <u>1966</u>, pp. 145-152 (unpublished); W. H. Miller, J. Chem. Phys. <u>51</u>, 3631 (1969); G. Vollmer, Z. Physik 226, 423 (1969).

⁵One may think: So does also any method yielding only one solution where an infinity of solutions hold. This is right, but the mathematically well-defined inverse methods enable one to get an appraisal of the range of all the solutions. Other methods cannot.

⁶T. Regge, Nuovo Cimento <u>14</u>, 951 (1949).

rivative in the input potential is too large, and are larger if the energy is smaller. This agrees perfectly, of course, with the filter effect of Eq. (19). Oscillations also appear in the tail, recalling the asymptotic behavior of the Bessel function in (1). The points below 0.5 F are in general not given; there is in most cases, close to the origin, a divergence $\sim r^{-1}$, due to (13). On the whole – except for badly discontinuous potentials – the surface range is fairly well reproduced; this agrees with the remarks made by many experimentalists concerning the sensitivity of scattering results to this part of the potential.¹⁸

⁷R. G. Newton, J. Math. Phys. <u>3</u>, 75 (1962); P. C. Sabatier, *ibid.* <u>7</u>, 1515 (1966); <u>7</u>, 2079 (1966).

⁸P. C. Sabatier, J. Math. Phys. <u>8</u>, 905 (1967).

⁹J. J. Loeffel, Ann. Inst. Henri Poincaré <u>8</u>, 339 (1968). ¹⁰A. Martin and G. Y. Targonski, Nuovo Cimento <u>20</u>, 1182 (1961).

¹¹G. A. Viano, Nuovo Cimento 63A, 581 (1969).

¹²P. C. Sabatier, Compt, Rend. <u>265</u>, 5 (1967).

¹³P.C. Sabatier (unpublished).

¹⁴F. Quyen Van Phu, Phys. Theor. Thesis, Montpellier University, 1970 (unpublished).

¹⁵The last ones are in most cases completely negligible. ¹⁶No effort has been made to meet typical experimental situations, because they are so varied. However, the whole numerical method is available in Ref. 14 and can easily be used to check the reliability in any design.

¹⁷It should be borne in mind that term "reliable" or "not reliable" does not mean here that the potential is, or is not, consistent with the experimental results; all the equivalent potentials are equally consistent with the experimental results.

¹⁸In Ref. 14, a figure is also given, showing that, for large values of r, the potential obtained through Newton's method show, in general, oscillations, obviously related to the expansion (1) of f(r, r').