Optical potentials from the scattering cross section by inversion

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The experimental elastic scattering cross section is inverted into an optical potential using a rational parametrization of the scattering function. A regularized error analysis is carried out. The method is successfully applied to the system α-^{40}Ca at 104 MeV.

I. INTRODUCTION

Empirical optical potentials are usually inferred from experimental elastic differential cross sections by search on the parameters of an assumed parametrized potential shape. The traditional search procedure based on the Woods-Saxon shape has in the recent past been extended or modified with the aim of making it more "model independent." We mention here the (Woods-Saxon)$^{\nu}$ fits,[1] the Fourier-Bessel expansion,[2] the orthogonal polynomial expansion,[3] the sum-of-Gaussians method,[4] and the cubic spline fits.[5–7]

While it is impossible to determine the potential deductively from the cross section with the help of some analytic algorithm, this can in principle be done if the input is not the cross section but the scattering function (or its logarithm, the phase shift). The latter is the inverse scattering problem at fixed energy: calculating the potential from the phase shifts as a function of angular momentum.[8–12]

In a recently proposed inversion method at fixed energy[13–15] the scattering function is interpolated by a rational function of angular momentum, whose poles and zeros determine uniquely the corresponding potential. This method has been applied in nuclear and atomic scattering.[16–19] Inasmuch as the rational interpolation of the scattering function between the integer angular momenta can be regarded as model independent, the same can then be said of the potential derived from this interpolation. A general discussion of potentials connected with simple classes of scattering functions is given in Refs. 20 and 21.

The input for the inverse scattering problem, the scattering function S_l at integer angular momenta $l=0,1,2,\ldots$, would have to be obtained from the experimental elastic cross section by a phase shift analysis (as in Ref. 22). For high energies and heavy particles, for example in heavy-ion scattering, a phase shift analysis which treats each phase shift independently, becomes forbiddingly difficult owing to the large number of phase shifts δ_l involved (one for each integer angular momentum l which contributes to the scattering). It appears much simpler to skip fitting the phase shifts: that is, to fit directly the small number of parameters $\mathbf{a}$ (poles and zeros) in the rational scattering function $S(l,\mathbf{a})$, to the experimental cross section.

This "rational scattering function analysis" of the cross section is not only more practical than the traditional phase shift analysis, it has the further great advantage of yielding immediately the associated scattering potential via the algorithm of Ref. 15. Although a search on the parameters $\mathbf{a}$ has to be made—this is no "deductive" procedure— and although a certain functional dependence of the phase shift δ_l on l is implied (though a rather flexible one), this procedure may perhaps be called a model independent inversion of the elastic cross section into the associated potential.

In the inversion the spread of the experimental data as well as the inaccuracies in the fitting procedure will induce errors in the potential.[23,24] Unless only a very few parameters $\mathbf{a}$ are used in the fit, the inverse problem will become an ill-posed problem, leading to large, unphysical errors in the potential. This can be remedied by a statistical regularization procedure.[25,26]

In the present paper we formulate such an inversion scheme for the cross section and apply it to a realistic case. In the next section, the inversion algorithm for a rational scattering function is briefly recalled, and the fitting of the parameters of this scattering function to the experimental cross section is explained. Section III is devoted to the derivation of the errors or confidence limits of the potential, and to a discussion of the regularization of the inversion procedure. In Sec. IV the method is applied to the scattering of α particles on ^{40}Ca at 104 MeV, and the results are compared with those of Ref. 27. Section V contains a summary.

II. INVERSION METHOD

The method[13–15] makes use of the fact that certain simple classes of scattering functions $S_l=S(l;\mathbf{a})$ charac-

terized by a finite number of parameters $\mathbf{a}=\{a_n\}$ are associated with certain easily calculable, analytic classes of local potentials. The determination of the potential ("inversion") then consists in determining the parameters $\mathbf{a}$ from the input scattering information [the scattering function S_l at $l=0,1,2,\ldots$ in the conventional inverse scattering problem or, as in the present work, the cross section $\sigma(\theta)$ at a finite number of angles $\theta=\theta_i$] by a fitting procedure. Thereafter, the potential is obtained automatically, as a by-product as it were. The search in the fit is on the parameters of the scattering function, not of the potential.

Examples of such classes are the *rational scattering function*[13]

$$S_{\text{rat}}(l;\mathbf{a})=S^{(0)}(\lambda)\prod_{n=1}^{N}\frac{\lambda^2-\beta_n^2}{\lambda^2-\alpha_n^2}\ , \tag{2.1}$$

where $\lambda=l+\frac{1}{2}$ and $\mathbf{a}=\{a_n\}=\{\alpha_n,\beta_n\}$, and $S^{(0)}(\lambda)$ is the scattering function of a possible reference potential $V_0(r)$, e.g., a Coulomb background potential; the *nonrational scattering function*[14]

$$S_{\text{nonrat}}(l;\mathbf{a})=S^{(0)}(\lambda)\frac{\left|\left|\dfrac{\sigma^{(0)}_{\beta_n}-\sigma^{(0)}_{\alpha_m}}{\beta_n^2-\alpha_m^2}-\dfrac{\sigma^{(0)}_{\lambda}-\sigma^{(0)}_{\alpha_m}}{\lambda^2-\alpha_m^2}\dfrac{\sigma^{(0)}_{\beta_n}}{\sigma^{(0)}_{\lambda}}\right|\right|}{\left|\left|\dfrac{\sigma^{(0)}_{\beta_n}-\sigma^{(0)}_{\alpha_m}}{\beta_n^2-\alpha_m^2}-\dfrac{\sigma^{(0)}_{\lambda}-\sigma^{(0)}_{\alpha_m}}{\lambda^2-\alpha_m^2}\right|\right|} \tag{2.2}$$

with $n,m=1,\ldots,N$ and

$$\sigma^{(0)}_{\lambda}=e^{-i\pi(\lambda-1/2)}S^{(0)}(\lambda)\ ;$$

and the "*mixed*" *scattering function,*[15] which is a product of expressions (2.1) and (2.2). Since the rational function can only be used when $\text{Im}\alpha_n^2>0$ and $\text{Im}\beta_n^2<0$,[14] while the nonrational function is appropriate only if $|\,\text{Im}\alpha_n\,|$, $|\,\text{Im}\beta_n\,|$ are reasonably large,[15] the mixed scheme must generally be employed.

The potential associated with these scattering functions is given by

$$V(r)=V_N(r)\ ; \tag{2.3}$$

$$V_n(r)=V_{n-1}(r)+V^{(n)}(r);\quad n-1,\ldots,N\ ; \tag{2.4}$$

$$V^{(n)}(r)=\frac{2}{r}(\beta_n^2-\alpha_n^2)\frac{d}{dr}\left[\frac{1}{r}\frac{1}{L^{(n-1)}_{\beta_n}(r)-L^{(n-1)}_{\alpha_n}(r)}\right]\cdot \tag{2.5}$$

The $L^{(n)\pm}_{\lambda}(r)$ are the logarithmic derivatives of the Jost solutions $f^{(n)\pm}_{\lambda}(r)$ to the potential $V_n(r)$ in the rational scheme, and of the regular solution $\phi^{(n)}_{\lambda}(r)$, in the nonrational scheme.[14,15]

A given set of S_l, $l=0,1,\ldots$, is easily interpolated by the rational function (2.1). The parameters $\mathbf{a}=\{\alpha_n,\beta_n\}$ are determined by setting

$$\prod_{n=1}^{N}(\lambda^2-\alpha_n^2)=\sum_{n=1}^{N}A_n\lambda^{2n-2}+\lambda^{2N}\ , \tag{2.6a}$$

$$\prod_{n=1}^{N}(\lambda^2-\beta_n^2)=\sum_{n=1}^{N}B_n\lambda^{2n-2}+\lambda^{2N}\ , \tag{2.6b}$$

and minimizing

$$\sum_{i=1}^{M}g_i\left[S_{li}\left[\sum_{n=1}^{N}A_n\lambda_i^{2n-2}+\lambda_i^{2N}\right]-S^{(0)}(\lambda_i)\left[\sum_{n=1}^{N}B_n\lambda_i^{2n-2}+\lambda_i^{2N}\right]\right]^2 \tag{2.7}$$

with respect to the $2N$ complex parameters A_n and B_n, $n=1,\ldots,N$. The number of fitting points is equal to $M\geqq 2N$, and the g_i are suitable weights. The minimization of expression (2.7) leads to a system of $2N$ linear equations with a unique solution for the coefficients A_n and B_n. From these the poles α_n^2 and zeros β_n^2 are found immediately. With the convention that all $\text{Im}\alpha_n<0$ and all $\text{Im}\beta_n>0$, we find that for $\text{Re}\alpha_n$, $\text{Re}\beta_n<0$ we have genuine Regge poles and zeros, while for $\text{Re}\alpha_n$, $\text{Re}\beta_n>0$ we have false Regge poles and zeros.[14] The former are taken into account in the rational form (2.1), and the latter in the nonrational form (2.2), with the condition that the imaginary parts of the false poles and zeros are sufficiently large ($\geqq 2$). The potential is then calculated as explained in Ref. 15.

Thus, the inversion starting from the scattering function S_l involves a unique "best" interpolation which is readily found by solving a linear system of equations. On the other hand, the inversion starting from the experimental *cross section* $\sigma(\theta)$ is not so straightforward. Here we introduce a "rational" cross section interpolation,

$$\sigma(\theta;\mathbf{a})=|\,f(\theta;\mathbf{a})\,|^2\ , \tag{2.8}$$

$$f(\theta;\mathbf{a})=f_{\text{Coul}}(\theta)+(2ik)^{-1}\sum_{l=0}^{\infty}(2l+1)[S_{\text{rat}}(l;\mathbf{a})-e^{2i\sigma_l}]P_l(\cos\theta)\ , \tag{2.9}$$

where $f_{\text{Coul}}(\theta)$ and σ_l are the Coulomb amplitude and phases, respectively. The parameters $\mathbf{a}=\{a_n\}=\{\alpha_n,\beta_n\}$ are determined by minimizing the sum of least squares

$$\chi^2(\boldsymbol{\sigma};\mathbf{a})\equiv\sum_{i=1}^{M}[\sigma_i-\sigma(\theta_i;\mathbf{a})]^2/(\Delta\sigma_i)^2\ , \tag{2.10}$$

where $\boldsymbol{\sigma}=\{\sigma_i\}=\{\sigma(\theta_i)\}$, and the θ_i are the measurement angles; $\Delta\sigma_i$ is the experimental error of σ_i.

Here the minimization problem does not lead to linear equations, but a nonlinear search on the $4N$ real parameters $\mathbf{a}$ must be made instead. This is unavoidable in any scheme: The cross section can in general be analyzed only by a search procedure, be it on the phase shifts, or on the poles or zeros of the rational scattering function. As mentioned in the Introduction, we regard the latter as more practicable than the former, quite apart from its "invertibility" into a potential. The search on the parameters $\mathbf{a}$ must be started with some starting values $\mathbf{a}^{(a)}$. These may be obtained by a rough Woods-Saxon–type fit of the cross section $\sigma(\theta)$, whereupon the scattering function S_l of that Woods-Saxon–type potential is used to calculate the parameters $\mathbf{a}^{(a)}$ from the linear equation discussed earlier.

We remark that a rational parametrization of the cross section of the type (2.8) has first been proposed by Remler.[28]

III. ERROR AND REGULARIZATION

Regarding the experimental errors as purely statistical, in particular, assuming that the experimental cross section values σ_i are independent stochastic variables with a normal distribution of variance $(\Delta\sigma_i)^2$, then[24,25]

$$P(\boldsymbol{\sigma}\mid\mathbf{a})=\text{const}\exp[-(\tfrac{1}{2})\chi^2(\boldsymbol{\sigma};\mathbf{a})] \tag{3.1}$$

is the conditional probability for σ_i if the "true" cross section is given by the expression (2.8) with some fixed but unknown parameters $\mathbf{a}$. One finds estimates $\hat{\mathbf{a}}$ of these parameters in terms of the experimental quantities σ_i, $(\Delta\sigma_i)^2$ by maximizing the probability (3.1), i.e., minimizing the function $\chi^2(\boldsymbol{\sigma};\mathbf{a})$ with respect to the variables $\mathbf{a}$ (as was indeed the recipe of the previous section). The minimum value is then given by

$$\chi^2_{\min}(\boldsymbol{\sigma})=\chi^2(\boldsymbol{\sigma};\hat{\mathbf{a}})\ ; \tag{3.2}$$

its expectation value over the distribution $P(\boldsymbol{\sigma}\mid\mathbf{a})$ of the variables $\boldsymbol{\sigma}$, is[25]

$$\overline{\chi^2_{\min}}=F\ , \tag{3.3}$$

where $F=M-4N$ is equal to the number of degrees of freedom.

In practice, the parametrized cross section (2.8) will not, in general, represent the true cross section exactly (although it might get quite close with sufficiently many parameters $\mathbf{a}$). Then, Eq. (3.3) is to be replaced by

$$\overline{\chi^2_{\min}}\gtrsim F\ . \tag{3.4}$$

Thus,

$$f=f(\boldsymbol{\sigma};\hat{\mathbf{a}})\equiv\chi^2(\boldsymbol{\sigma};\hat{\mathbf{a}})/F \tag{3.5}$$

is an estimate of the goodness of fit, the true fit giving $f=1$ on the average.

We now regard expression (3.1) as a distribution in the parameters $\mathbf{a}$ for given experimental values $\boldsymbol{\sigma}$, and define the average over a function $F(\mathbf{a})$,

$$\langle F(\mathbf{a})\rangle\equiv\int F(\mathbf{a})P(\boldsymbol{\sigma}\mid\mathbf{a})d\mathbf{a}\Big/\int P(\boldsymbol{\sigma}\mid\mathbf{a})d\mathbf{a}\ . \tag{3.6}$$

Then, the covariance of the parameters $\mathbf{a}$ defines the error matrix[25] $(\Delta a_n=a_n-a_n)$

$$\epsilon_{nm}\equiv\langle\Delta a_n\Delta a_m\rangle=\alpha^{-1}_{nm}f\ . \tag{3.7}$$

Here,

$$\alpha_{nm}=\frac{1}{2}\frac{\partial^2\chi^2}{\partial a_n\partial a_m}\bigg|_{\hat{\mathbf{a}}}=\sum_{i=1}^{M}\frac{\partial\sigma(\theta_i;\mathbf{a})}{\partial a_n}\frac{\partial\sigma(\theta_i;\mathbf{a})}{\partial a_m}\bigg|_{\hat{\mathbf{a}}}\frac{1}{(\Delta\sigma_i)^2} \tag{3.8}$$

is the curvature, or normal matrix, and the parabolic approximation is assumed valid near the minimum of χ^2.

This yields for the covariance of the potential $V(r)=V(r;\hat{\mathbf{a}})$,

$$\langle\Delta V(r)\Delta V(r')\rangle=\sum_{n,m=1}^{4N}\frac{\partial V(r)}{\partial a_n}\frac{\partial V(r')}{\partial a_m}\bigg|_{\hat{\mathbf{a}}}\epsilon_{nm}\ . \tag{3.9}$$

Thus, we have for the error

$$[\overline{\Delta V(r)}]^2\equiv\langle[\Delta V(r)]^2\rangle=\sum_{n,m=1}^{4N}\frac{\partial V(r)}{\partial a_n}\frac{\partial V(r)}{\partial a_m}\bigg|_{\hat{\mathbf{a}}}\epsilon_{nm}\ . \tag{3.10}$$

If the potential is complex, Eq. (3.9) is to be generalized to a covariance for the real and imaginary parts, and Eq. (3.10) holds for $\mathrm{Re}\,V(r)$ and $\mathrm{Im}\,V(r)$ separately. We remark that one could analogously define the covariance for the scattering function $S(\lambda)$, and make an error analysis on the phase shifts in terms of our rational parametrization.

The fit to the experimental cross section will generally be the better (i.e., f will be the closer to unity) the larger the number $4N$ of parameters. But as N increases, the normal matrix α_{nm} becomes ill conditioned,[26,29] and the errors $\overline{\Delta V(r)}$ will become very large. A family of highly fluctuating, unphysical potentials will be found which, however, all give rise to fits of the cross section $\sigma(\theta)$ within the experimental errors.

By keeping the number of parameters low, the class of potentials can be kept "smooth," at the possible expense of the goodness of fit. This has been called "parametric regularization."[20] A more satisfying method is the statistical regularization scheme,[26] which has been introduced in nuclear scattering by Krappe and Rossner.[29] (Another method of regularization is that of Ref. 30.) As applied to the present situation, the method stipulates that the searched-for potential be as close to a pregiven *a priori* potential "as the experimental data allow." Since the potential is determined by the parameters $\mathbf{a}$, we consider an equivalent set of *a priori* parameters $\mathbf{a}^{(a)}$, which, as the notation indicates, are conveniently identified with the starting values of the parameter search. These *a priori* parameters determined a normal *a priori* distribution with assumed variance $1/\gamma$:[26]

$$P_{a\ priori}(\mathbf{a})=\text{const}\exp[-(\gamma/2)\sum_{n=1}^{4N}(a_n-a_n^{(a)})^2]\ . \tag{3.11}$$

Together with the experimental information described by the distribution $P(\boldsymbol{\sigma}\mid\mathbf{a})$ of Eq. (3.1) we have the *a posteriori* distribution (Bayes formula)

$$P_{a\ post}(\mathbf{a}\mid\boldsymbol{\sigma})=\frac{P_{a\ priori}(\mathbf{a})P(\boldsymbol{\sigma}\mid\mathbf{a})}{\int P_{a\ priori}(\mathbf{a})P(\boldsymbol{\sigma}\mid\mathbf{a})d\mathbf{a}}\ . \tag{3.12}$$

This conditional probability in the parameters $\mathbf{a}$, for given values $\boldsymbol{\sigma}$, is to be maximized to yield estimates for the *a posteriori* parameters $\mathbf{a}$. That is, one must determine the minimum of the expression

$$\tilde{\chi}^2(\boldsymbol{\sigma};\mathbf{a})\equiv\gamma\sum_{n=1}^{4N}(a_n-a_n^{(a)})^2+\chi^2(\boldsymbol{\sigma};\mathbf{a}) \tag{3.13}$$

with respect to the variables a_n, which results in the *a posteriori* estimate $\hat{\mathbf{a}}(\gamma)=\{a_n(\gamma)\}$.

For $\gamma=0$ we obtain the previous goodness-of-fit value f of Eq. (3.3) without *a priori* information; as γ increases, the value of

$$f(\gamma)\equiv\chi^2(\sigma;\hat{\mathbf{a}}(\gamma))/F \tag{3.14}$$

increases as well, i.e., the fit gets worse. However, the regularized error matrix[26,29]

$$\epsilon_{nm}(\gamma)=[\beta(\gamma)^{-1}]_{nm}f(\gamma)\ , \tag{3.15}$$

where

$$\beta_{nm}(\gamma)=\alpha_{nm}(\gamma)+\gamma\delta_{nm} \tag{3.16}$$

and $\alpha_{nm}(\gamma)$ is α_{nm} of Eq. (3.8) evaluated at $\hat{\mathbf{a}}(\gamma)$, has reduced, stabilized matrix elements, and the errors of the potential cease to be fluctuating between large limits.

As to the value of γ, i.e., the degree to which the *a priori* information is taken into account, one may require that it be chosen such that the value of the function $\chi^2_{\min}(\gamma)\equiv\chi^2(\sigma;\hat{\mathbf{a}}(\gamma))$ associated with the minimum value of $\tilde{\chi}^2$, $\tilde{\chi}^2_{\min}=\tilde{\chi}^2(\sigma;\hat{\mathbf{a}}(\gamma))$, be equal to the unregularized average value of χ^2 (Philipps condition):[31]

$$\chi^2_{\min}(\gamma)=\langle\chi^2\rangle\ . \tag{3.17}$$

Thus, one allows the *a posteriori* "*minimum*" $\chi^2(\gamma)$ value to be as large as the unregularized, "unbiased" *average* χ^2 value $\langle\chi^2\rangle>\chi^2_{\min}$.

Alternatively, one may require that the *a posteriori average* of χ^2 be equal to the unregularized average of χ^2 (Turchin condition):[26]

$$\langle\chi^2\rangle_{a\ post}=\langle\chi^2\rangle\ , \tag{3.18}$$

where

$$\langle\chi^2\rangle_{a\ post}\equiv\int\chi^2(\sigma;\mathbf{a})P_{a\ post}(\mathbf{a}\mid\sigma)d\mathbf{a}\ . \tag{3.19}$$

This last condition gives less weight to the *a priori* information than the former.

Now[26]

$$\begin{aligned}\langle\chi^2\rangle&=\chi^2_{\min}+4N\ ,\\ \langle\chi^2\rangle_{a\ post}&=\chi^2_{\min}(\gamma)+4N_{\rm eff}(\gamma)\ ,\end{aligned} \tag{3.20}$$

where

$$4N_{\rm eff}(\gamma)=\sum_{n,m}^{4N}\epsilon_{nm}(\gamma)\alpha_{nm}(\gamma)\,|_{\hat{\mathbf{a}}(\gamma)} \tag{3.21}$$

is the effective number of parameters $[4N_{\rm eff}(0)=4N]$. Therefore, condition (3.17) implies (Philipps)

$$\chi^2_{\min}(\gamma)=\chi^2_{\min}+4N\ , \tag{3.22}$$

while condition (3.18) means (Turchin)

$$\chi^2_{\min}(\gamma)+4N_{\rm eff}(\gamma)=\chi^2_{\min}+4N\ . \tag{3.23}$$

In either case, one starts with a large value of γ, when the left-hand sides are larger than the right-hand sides, and reduces it until Eqs. (3.22) and (3.23) are satisfied.

IV. APPLICATION TO α-^{40}Ca AT 104 MeV

A. Data and *a priori* potential

For a demonstration of the method, we "invert" the elastic cross section data of Gils *et al.*[27] for α on ^{40}Ca at 104 MeV, since these authors appear to provide the best available data which, moreover, they have fitted by a potential using the Fourier-Bessel method. These data are shown in Figs. 4 and 5. Gils *et al.*[27] have made a "rough" fit to these with a Woods-Saxon potential with parameters $V=151.9$ MeV, $r_{01}=1.407$ fm, $a_1=1.248$ fm (real form factor squared), and $W=20.3$ MeV, $r_{02}=1.607$ fm, $a_2=0.672$ fm, $R_i=r_{0i}A^{1/3}$, plus a double-folding Coulomb potential[27] (this is fairly close to a charged-sphere potential). This rough fit achieves a goodness of fit value $f=3.3$

The scattering function calculated with this potential can be very accurately fitted (at $M=80$ angular momenta l_i) by a rational scattering function of the form (2.1) with

$$S^{(0)}(\lambda)=e^{i\eta\ln(\lambda^2+\lambda_c^2)} \tag{4.1}$$

corresponding to a Coulomb reference function[15] with $\eta=40$ $e^2/\hbar v=1.2354$, $\lambda_c=8\eta$, and the $4N=32$ real parameters $\mathbf{a}^{(a)}=\{\alpha_n^{(a)},\beta_n^{(a)}\}$ given in Table I. (We remark that for convenience two zeros β_n are taken into account in the nonrational form although they should be counted as rational according to Sec. II.)

TABLE I. *A priori* parameters ("$\gamma\to\infty$").

	n	α_n	β_n
Nonrational	1	15.839 20 − i 25.214 40	24.640 80 + i 11.582 00
	2	24.449 70 − i 11.318 20	−18.037 00 + i 18.370 20
	3	20.101 40 − i 6.589 27	− 4.119 30 + i 5.642 55
Rational	4	− 8.349 48 − i 7.869 54	−21.313 70 + i 0.424 03
	5	−23.037 60 − i 5.095 80	−19.209 90 + i 1.354 63
	6	−10.959 10 − i 4.898 35	−16.781 200 + i 2.221 91
	7	−18.684 50 − i 7.709 72	−13.715 00 + i 3.170 24
	8	−14.862 30 − i 6.346 00	− 9.616 02 + i 4.311 02

B. Search for the optimal parameters

Starting with the parameters $\mathbf{a}^{(a)}$, with γ fixed at various values between 0 and 10.0, a search is made on the parameters $\mathbf{a}$ to find the minimum of the function $\tilde{\chi}^2(\sigma;\mathbf{a})$ of Eq. (3.13), using $M=140$ scattering angles θ_i. This search is carried out with the help of the program INBAFI,[32] which is based on the Marquardt algorithm.[33] In the search the signs of the real and imaginary parts of the parameters were kept fixed at their *a priori* values. The minimum value found, $\tilde{\chi}^2_{\min}(\gamma)=\tilde{\chi}^2(\sigma;\hat{\mathbf{a}}(\gamma))$, is plotted as a function of γ in Fig. 1(a); the corresponding functions $\chi^2_{\min}(\gamma)=\chi^2(\sigma;\hat{\mathbf{a}}(\gamma))$, $\langle\chi^2\rangle_{a\ post}$, and $4N_{\text{eff}}(\gamma)$ are displayed in Figs. 1(b)–(d), respectively.

It is seen that, unfortunately, the search program does not always yield a unique minimum; rather, in various regions of γ, different families of solutions yield the lowest minimum. For the fulfillment of the Philipps condition (3.17) [cf. Fig. 1(b)] we choose family 2 because family 3 yields no solution, and there is no corresponding local

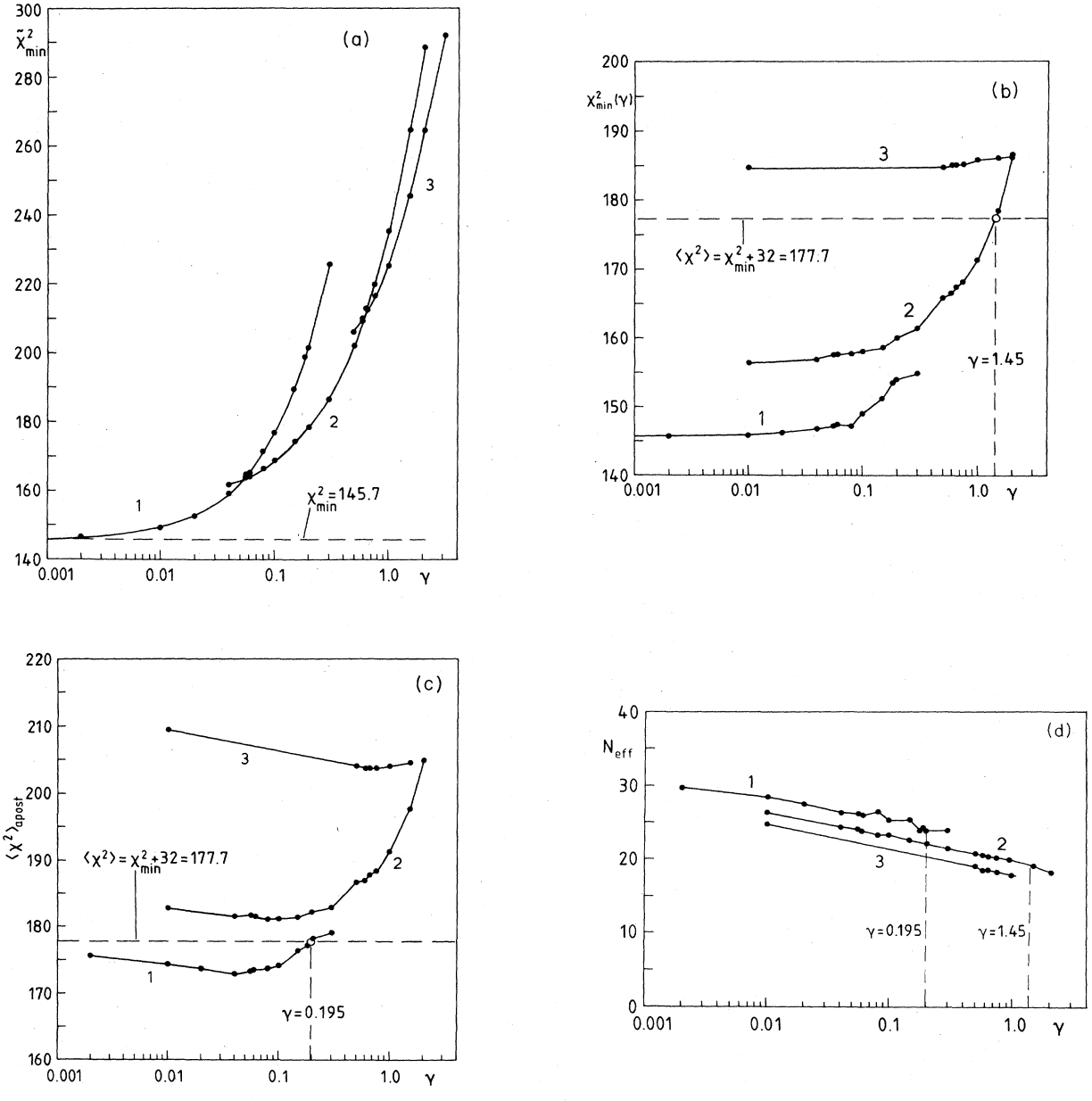

FIG. 1. (a) The minimum value $\tilde{\chi}^2_{\min}(\gamma)$ determined by search on the parameters $\mathbf{a}$ at fixed γ. Three different families are found by varying the starting values of $\mathbf{a}$ for different γ. (b) The function $\chi^2_{\min}(\gamma)$ associated with the minimum value $\tilde{\chi}^2_{\min}(\gamma)$. The intersection with $\langle\chi^2\rangle=177.7$ yields the "Philipps value" $\gamma=1.45$. (c) The *a posteriori* average $\langle\chi^2\rangle_{a\ post}$ associated with the minimum value $\tilde{\chi}^2(\gamma)$. The intersection with $\langle\chi^2\rangle=177.7$ yields the "Turchin value" $\gamma=0.195$. (d) The effective number of parameters $N_{\text{eff}}(\gamma)$ associated with the minimum value $\tilde{\chi}^2(\gamma)$.

TABLE II. Optimal parameters for condition (3.22) ($\gamma=1.45$).

	n	α_n	β_n
	1	15.668 60 − i 25.595 90	27.321 80 + i 10.476 10
Nonrational	2	25.059 60 − i 11.248 40	−18.281 20 + i 18.372 90
	3	19.863 10 − i 6.126 95	− 3.310 99 + i 5.346 60
	4	− 9.073 68 − i 4.365 67	−20.600 50 + i 1.431 51
	5	−25.833 60 − i 7.487 36	−20.291 70 + i 2.680 98
Rational	6	−19.125 20 − i 4.025 79	−15.528 30 + i 0.596 20
	7	−16.918 40 − i 7.557 36	−12.209 50 + i 2.870 75
	8	−14.483 40 − i 5.216 21	− 8.250 91 + i 4.034 62

minimum of $\tilde{\chi}^2$ related to family 1. This results in the value $\gamma=1.45$. For the fulfillment of the Turchin condition (3.18) [cf. Fig. 1(c)] only family 1 can be used, yielding the value $\gamma=0.195$. The parameters $\hat{\mathbf{a}}(\gamma)$ for these two solutions are given in Tables II and III.

C. The potentials

The potentials (2.3) calculated from the two sets of parameters are shown in Figs. 2 and 3, together with the errors $\overline{\Delta V(r)}$ calculated by formula (3.10); the error matrix ϵ_{nm} is here of course calculated with the help of Eq. (3.15). According to Fig. 9.2b of Ref. 24, the resulting error bands, or confidence intervals, correspond to a probability content of about 55% (number of parameters: $4N=32$). It is seen that the final potentials are significantly shifted away from their *a priori* shape.

The Philipps condition (3.17) yields a smoother potential, with smaller confidence intervals, than the Turchin condition (3.18). The price for this is a slightly worse fit (larger value of f). The fits to the cross section resulting from an inversion using the Philipps and Turchin conditions are shown in Figs. 4 and 5, respectively. To the eye they appear as equally perfect, although $f=1.675$ for the Philipps condition and $f=1.417$ for the Turchin condition. If no *a priori* information is used at all ($\gamma=0$) a fit with $f=1.35$ is obtained, which indicates that the rational scattering function with $4N=32$ real parameters is only just adequate statistically to describe the experimental cross section ($F=108$).[25] The corresponding unregularized potential, however, has errors which generally attain values of to 100% of the potential itself.

It is seen from Fig. 1(d) that the effective number of real parameters for the regularized fits is $4N_{\text{eff}}\approx 19$ for $\gamma=1.45$ and $4N_{\text{eff}}\approx 24$ for $\gamma=0.195$. That is, instead of the 32 real parameters introduced in the rational interpolation, one effectively needs only about 20 independent parameters in order to obtain acceptable fits to the cross section in the light of the assumed *a priori* information.

The regularized inversion of the high-quality α-^{40}Ca scattering cross section data[27] yields smooth potentials with fairly narrow confidence limits. The two potentials obtained by the two different methods of choosing an optimal value of γ are practically the same in the (physically important) surface region, but they differ in the interior. Owing to the absorption in this region, the actual value of the potential is not very important there, however. Nevertheless, the fact that the two potentials differ from one another outside their confidence limits would have to be attributed to a significant difference between the Philipps and Turchin conditions together with a certain (physically irrelevant) rigidity of the rational scattering function analysis (a certain "model dependence" showing up in unimportant parts of the potential, but not in the cross section). The choice of the *a priori* potential may of course also prejudice certain local $\tilde{\chi}^2$ minima. In the physically relevant surface region all these ambiguities are kept to a minimum.

TABLE III. Optimal parameters for condition (3.23) ($\gamma=0.195$).

	n	α_n	β_n
	1	14.183 80 − i 24.358 90	30.120 00 + i 6.935 93
Nonrational	2	24.580 90 − i 12.936 70	−19.373 10 + i 19.133 10
	3	19.237 90 − i 6.852 95	− 4.253 10 + i 5.781 43
	4	− 9.925 88 − i 6.198 39	−19.795 50 + i 0.001 62
	5	−29.101 20 − i 6.146 75	−21.727 10 + i 1.766 78
Rational	6	−21.939 00 − i 3.664 32	−15.698 40 + i 3.116 50
	7	−17.977 60 − i 4.309 60	−13.556 40 + i 0.001 12
	8	−12.281 70 − i 5.273 97	− 0.001 67 + i 3.998 07

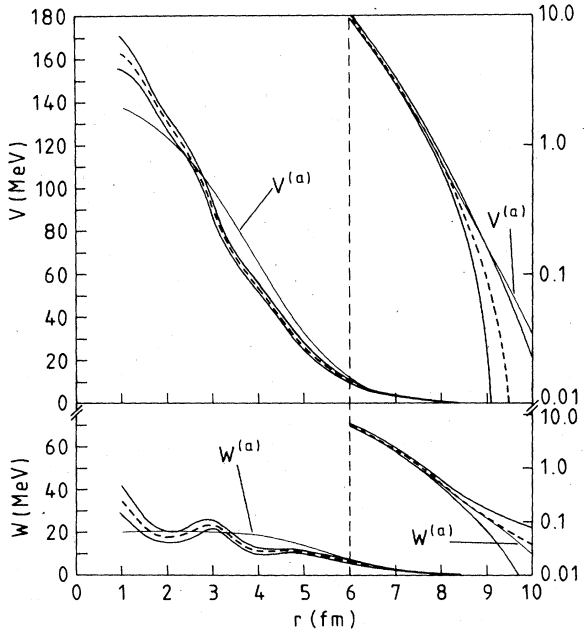

FIG. 2. The optical potential $-V-iW$ with confidence limits corresponding to probability content 55% for $\gamma=1.45$. Also shown is the *a priori* potential $-V^{(a)}-iW^{(a)}$.

Gils *et al.*[27] have also used their data to derive a potential by the Fourier-Bessel method. They keep the imaginary part of the potential fixed at the *a priori* Woods-Saxon shape, searching only on the Fourier-Bessel coefficients of the real part. Their fit results in a slightly larger f value than ours, $f=2.2$, and in a smoother real potential

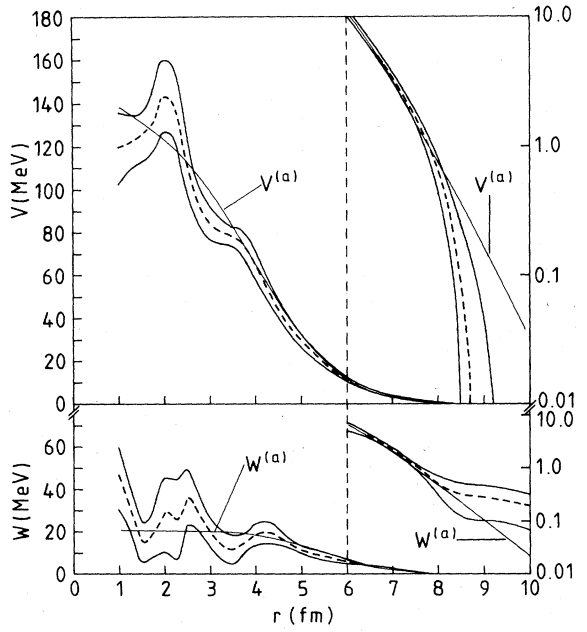

FIG. 3. Same as Fig. 2 for $\gamma=0.195$.

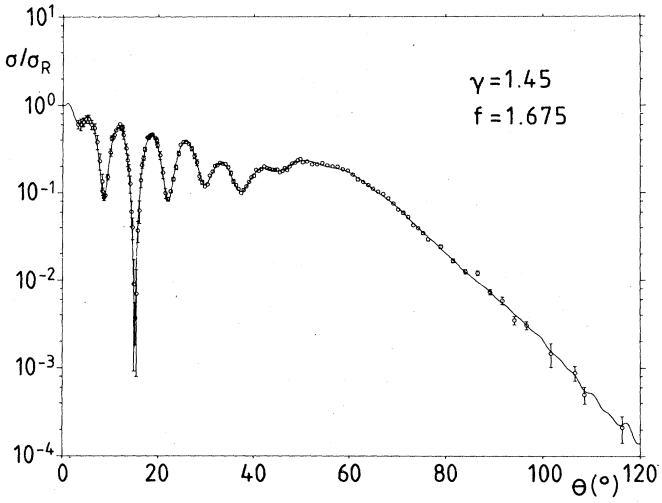

FIG. 4. Experimental elastic cross section and the rational fit for $\gamma=1.45$.

with narrower confidence limits. In the physically important surface region, both the real and imaginary parts of their potential are deeper than ours by more than their error limits. The small errors in their potential are apparently connected with the "parametric regularization" through the use of a low number (9—12) of free parameters in the Fourier-Bessel method. The discrepancies between the Fourier-Bessel potential and the ones obtained in the present work evidently stem from this difference in the number of free parameters.

V. CONCLUSION

From the present analysis it emerges that the inversion scheme based on a rational scattering function analysis of the experimental elastic cross section leads to reasonable results. This inversion method is not an analytic pro-

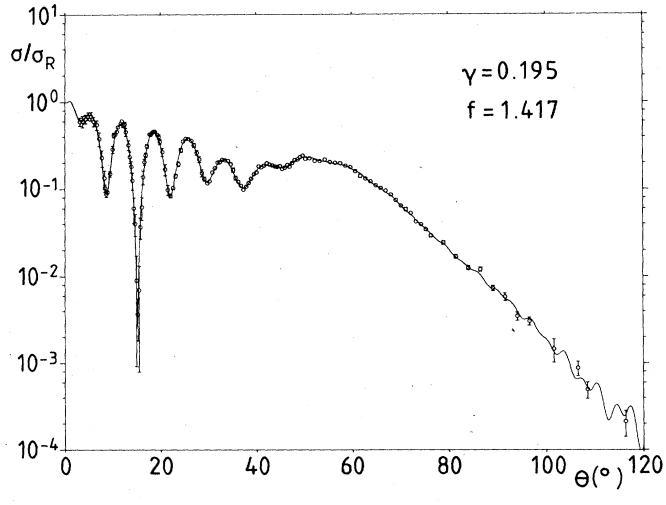

FIG. 5. Same as Fig. 4 for $\gamma=0.195$.

cedure, since it involves a parameter search in going from the cross section to the scattering function. But cross sections can in general be analyzed only by some search procedure; instead of the traditional phase shift search analysis we propose here the somewhat more restricted rational analysis, which involves less parameters, yet is apparently still flexible enough to represent realistic cross sections. The rational analysis automatically yields the corresponding potential, including confidence limits. The *a priori* parameters used in the present work are admittedly introduced *ad hoc* on the basis of reasonableness. A more model independent starting set would indeed be desirable. Further research should also deal with the problem of the occurrence of local minima. The method should facilitate the investigation of the sensitivity of the potential to the cross section in various angular regions.

[1]F. Michel and R. Vanderpoorten, Phys. Rev. C **16**, 142 (1977); H. P. Gubler, U. Kiebele, H. O. Meyer, G. R. Plattner, and I. Sick, Phys. Lett. **74B**, 202 (1978).
[2]E. Friedman and C. J. Batty, Phys. Rev. C **17**, 34 (1978).
[3]P. L. Roberson, Phys. Rev. C **22**, 482 (1980).
[4]H. P. Gubler, U. Kiebele, H. O. Meyer, G. R. Plattner, and I. Sick, Nucl. Phys. **A351**, 29 (1981).
[5]L. W. Put and A. M. J. Paans, Nucl. Phys. **A291**, 93 (1977).
[6]F. Michel and R. Vanderpoorten, Phys. Lett. **82B**, 183 (1979).
[7]A. M. Kobos and R. S. Mackintosh, Ann. Phys. (N.Y.) **123**, 296 (1979); Phys. Lett. **92B**, 59 (1980).
[8]R. G. Newton, J. Math. Phys. **3**, 73 (1962); **8**, 1566 (1967).
[9]P. C. Sabatier, J. Math. Phys. **7**, 1515 (1966); **7**, 2079 (1966); **8**, 905 (1967); **9**, 1241 (1968).
[10]C. Coudray, Lett. Nuovo Cimento **19**, 319 (1977).
[11]M. Münchow and W. Scheid, Phys. Rev. Lett. **44**, 1299 (1980); K. E. May, M. Münchow, and W. Scheid, Phys. Lett. **141B**, 1 (1984).
[12]R. A. Baldock, B. A. Robson, and R. F. Barrett, Nucl. Phys. **A366**, 270 (1981).
[13]R. Lipperheide and H. Fiedeldey, Z. Phys. A **286**, 45 (1978).
[14]R. Lipperheide and H. Fiedeldey, Z. Phys. A **301**, 81 (1981).
[15]K. Naidoo, H. Fiedeldey, S. A. Sofianos, and R. Lipperheide, Nucl. Phys. **A419**, 13 (1984).
[16]R. Lipperheide, H. Fiedeldey, H. Haberzettl, and K. Naidoo, Phys. Lett. **82B**, 39 (1979).
[17]P. Fröbrich, R. Lipperheide, and H. Fiedeldey, Phys. Rev. Lett. **43**, 1147 (1979).
[18]R. Lipperheide, S. Sofianos, and H. Fiedeldey, Phys. Rev. C **26**, 770 (1982).
[19]H. Bürger, L. J. Allan, H. Fiedeldey, S. A. Sofianos, and R. Lipperheide, Phys. Lett. **97A**, 39 (1983).
[20]B. N. Zakhar'ev, V. N. Pivovarchik, E. B. Plekhanov, and A. A. Suz'ko, Fiz. Elem. Chastits At. Yadra **13**, 1284 (1982) [Sov. J. Part. Nuclei **13**, 535 (1982)].
[21]P. S. Sabatier, Laboratoire de Physique Mathématique, Montpellier, Report PM 84/13, 1984.
[22]A. A. Ioannides and R. S. Mackintosh, Nucl. Phys. **A438**, 354 (1985).
[23]D. W. O. Rogers, Nucl. Instrum. Methods **127**, 253 (1975).
[24]W. T. Eadie, D. Dryard, F. E. James, M. Roos, and B. Sadoulet, *Statistical Methods in Experimental Physics* (North-Holland, Amsterdam, 1971).
[25]P. R. Bevington, *Data Reduction and Error Analysis for the Physical Sciences* (McGraw-Hill, New York, 1975).
[26]V. F. Turchin, V. P. Kozlov, and M. S. Malkevich, Usp. Fiz. Nauk. **102**, 345 (1970) [Sov. Phys.—Usp. **13**, 681 (1971)].
[27]H. J. Gils, H. Rebel, and E. Friedman, Phys. Rev. C **29**, 1295 (1984).
[28]E. A. Remler, Phys. Rev. A **3**, 1949 (1971).
[29]H. J. Krappe and H. Rossner, Z. Phys. A **314**, 149 (1983).
[30]J. Borysowicz and J. H. Hetherington, Phys. Rev. C **7**, 2293 (1973).
[31]D. L. Philipps, J. Assoc. Comput. Mach. **9**, 84 (1962).
[32]H. Leeb, INBAFI, Technische Universität Wien, 1983.
[33]D. W. Marquardt, SIAM J. Appl. Math. **11**, 431 (1963).