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χ^2 or Δ test function in analysis of nuclear elastic scattering data

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The paper presents differences in the results of the optical-model analyses of nuclear elastic scattering data when the true χ^2 and its approximation, i.e., the Δ test functions, are used in an automatic search for the best model parameters.

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I. INTRODUCTION

Nuclear elastic scattering is the simplest nuclear process studied since the early beginning of nuclear physics. The main task when investigating this reaction is to develop a theoretical model that can describe it correctly. There are few such models, of classical, semiclassical, and pure quantum-mechanical nature. The commonly used quantum-mechanical model is the optical model (OM), in which elastic scattering differential cross sections are described as a result of the Coulomb and nuclear interactions of beam particles with the nucleus by use of a complex nuclear potential. However, the simple phenomenological spherical OM is not able to reproduce the experimental data perfectly, and it serves only as a starting point for its further modifications and extensions. Using this model, we adjust the parameters of the complex nuclear potential until the theoretical predictions are as close to the experimental data as possible. With a computer, the set of measured elastic cross sections $\sigma_{\rm el}(\theta_i)$ at angles θ_i, with their experimental errors $\delta\sigma_{\rm el}(\theta_i)$, is compared with the set of calculated theoretical cross sections $\sigma_{\rm th}(\theta_i)$ for the same scattering angles. The model parameters are adjusted until the best fit is obtained. The procedure used to determine the optimal set of parameters of the OM is called the automatic search routine. It is then necessary to choose a quantitative measure of a goodness-of-fit function that would stop the search when the theoretical predictions are as close to the experimental data as possible. The choice of a goodness-of-fit test function is to some extent arbitrary, but it must be statistically acceptable and should be the same for all research groups to allow a comparison of the fits' quality. As will be shown later, the goodness-of-fit test function used so far is probably not the best one, especially when fitting the nuclear elastic channel.

II. THE χ^2 AND Δ TEST FUNCTIONS

In statistics, there is a test function used to judge how good the theoretical predictions agree with a set of experimental data. This is the χ^2 test function, defined as

$$\chi^2 = \sum_{i=1}^{n} \frac{\left(N_T^i - N_E^i\right)^2}{N_T^i} \tag{1}$$

where N_E^i and N_T^i are the experimental and theoretical numbers for the ith measurement and summations run from 1 to n separate measurements. In the present situation N_E^i and N_T^i are the number of detected particles scattered through an angle θ_i and the predicted number of scattered particles through the same angle, respectively. However, we should compare, not the number of scattered particles, but the values of experimental and theoretical cross sections σ_E^i and σ_T^i. These are related to the numbers of scattered particles by very simple relations: $\sigma_T^i = \alpha N_T^i$ and $\sigma_E^i = \alpha N_E^i$. The experimental cross sections have the uncertainty $\delta\sigma_E^i = \alpha (N_E^i)^{1/2}$. From the preceding expression α can be expressed as $\alpha = (\delta\sigma_E^i)^2/\sigma_E^i$. Calculating N_E^i and N_T^i from the preceding relations and inserting these into Eq. (1), we can write it in the form presented by Hodgson in his book *The Optical Model of Elastic Scattering* [1], i.e., in the form

$$\chi^2 = \sum_{i=1}^{n} \left(\frac{\sigma_T^i - \sigma_E^i}{\delta\sigma_E^i}\right)^2 \frac{\sigma_E^i}{\sigma_T^i}. \tag{2}$$

Next Hodgson made an assumption that, if the theory is perfectly good, then $\sigma_E \simeq \sigma_T$, and therefore $\sigma_E/\sigma_T \simeq 1$, and he got

$$\Delta = \sum_{i=1}^{n} \left(\frac{\sigma_T^i - \sigma_E^i}{\delta\sigma_E^i}\right)^2 \simeq \chi^2. \tag{3}$$

This approximation is generally incorrect. This aproximation can be accepted only when the theory is perfectly good and when the ratios σ_E/σ_T are uniformely distributed around unity. We know that the OM is not a perfect theory and is unable to reproduce the experimental data perfectly, especially for strongly absorbed particles and heavy ions, and then σ_E/σ_T is not symmetrically distributed around unity. Moreover, Eq. (2) can be written in the form

$$\chi^2 = \sum_{i=1}^{n} \left(\frac{\sigma_E^i}{\delta\sigma_E^i}\right)^2 \left(\frac{\sigma_T^i}{\sigma_E^i} + \frac{\sigma_E^i}{\sigma_T^i} - 2\right), \tag{4}$$

where $\sigma_E^i/\delta\sigma_E^i$ is the reverse of the relative experimental error of the ith point. These fractions are playing the role of weighting coefficients for each experimental point in the total sum.

Now, if we put $\sigma_E/\sigma_T \simeq 1$, then we should put $\sigma_T/\sigma_E \simeq 1$ too!

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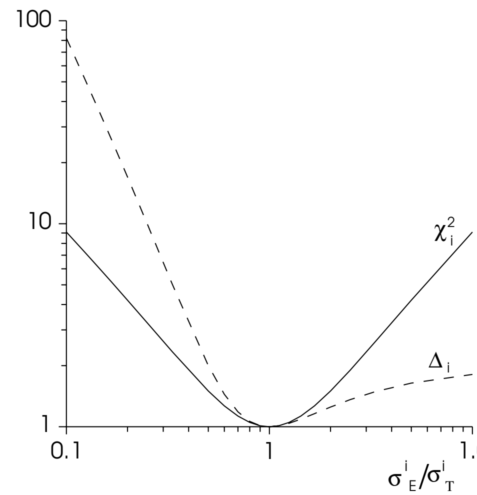

FIG. 1. Theoretical profiles of χ_i^2 (solid curve) and Δ_i (dashed curve) tests as functions of the σ_E^i/σ_T^i ratio.

We can also present Eq. (3) in the same form as that of Eq. (4), and thus we have

$$\Delta = \sum_{i=1}^{n} \left(\frac{\sigma_E^i}{\delta\sigma_E^i}\right)^2 \left(\frac{\sigma_T^i}{\sigma_E^i} - 1\right)^2 \tag{5}$$

We see then that χ^2 and Δ are completely different functions.

The Δ function (which in fact is a function of the least-squares method) has been adopted as an approximation of χ^2, and this function is widely used in all OM automatic search routines. Both functions, χ^2 and Δ, have minima at the same point (where all $\sigma_T^i = \sigma_E^i$) but, as shown in Fig. 1, the former is symmetric around the minimum, whereas the latter is highly asymmetric around it (note that the ratio σ_T^i/σ_E^i is plotted on a log scale). It is only in the nearest vicinity of the minimum that χ^2 can be approximated by the Δ function. As will be shown in the next section, both functions work in a slightly different way and give different search results.

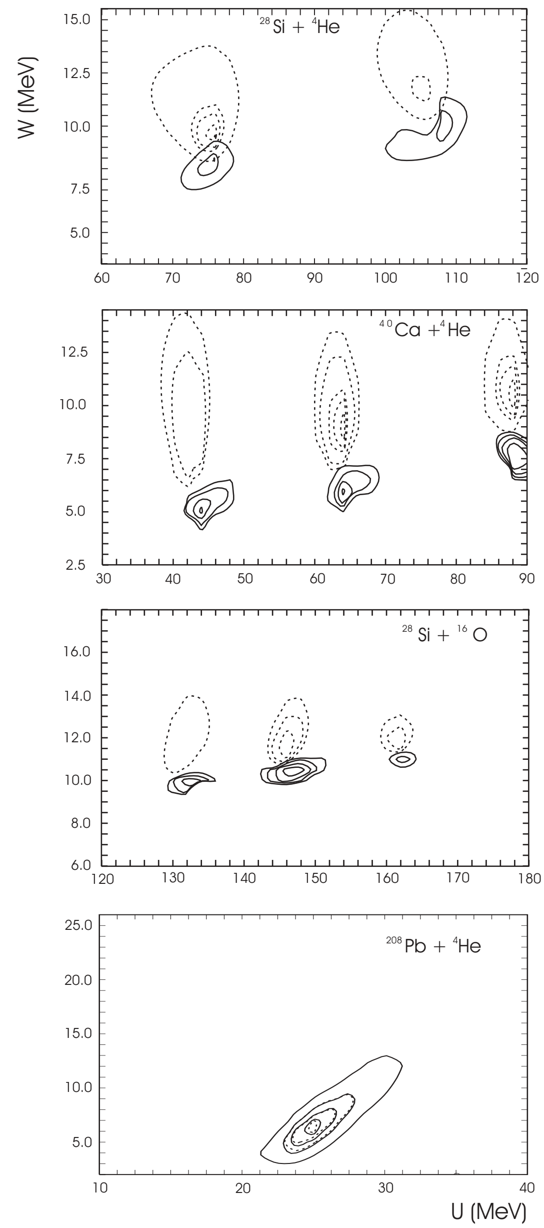

FIG. 2. The positions of minima of χ^2 (solid curves) and Δ (dashed curves) test functions found when they were scanned in the U - W space for a set of four experimental elastic scattering data.

III. THE χ^2 AND Δ SURFACES

To examine how both test functions work, we analyzed four low-energy experimental elastic scattering data, present in literature, by means of a four-parameter phenomenological OM by using both test functions. The selected data were $^{28}Si + {}^{4}He$ at 26.5 MeV [2], $^{40}Ca + {}^{4}He$ at 24.15 MeV [3], $^{28}Si + {}^{16}O$ at 54.69 MeV [4], and $^{208}Pb + {}^{4}He$ at 26.0 Mev [5]. The analysis was performed by a scan of the χ^2 and Δ surfaces in two-parameter space, i.e., in the U - W space with fixed geometrical parameters r_0 and a. The geometrical form factor for real and imaginary parts of the OM potentials was of the ordinary Woods-Saxon type, without surface absorption.

The positions of the minima obtained for the χ^2 and Δ functions are shown in Fig. 2. The exact positions of these minima are listed in Table I. The differences in the positions of the minima found for the χ^2 and Δ functions seem to be rather small, and for $^{208}Pb + {}^{4}He$ both minima are at the same position. For this case, we have one well-defined minimum and no "discrete" ambiguity. If we now calculate the angular distributions for these minima, we see a substantial difference in the differential cross section at backward angles for three sets of experimental data and no difference for $^{208}Pb + {}^{4}He$. The results are presented in Fig. 3. Looking at these results, we see that the differential cross sections at backward angles are much closer to the experimental data for the χ^2 minima than those for the Δ function. If we now perform a search of all four parameters within the minima found by scanning, we get sets of parameters that are almost identical to those presented in

TABLE I. OM parameters for the minima of χ^2 and Δ surfaces found when they were scanned in the U - W space for a set of four various experimental elastic scattering data. N is the number of experimental points. The values of inactive test functions in the last two columns are in parentheses.

Reaction	N	E_{lab} (MeV)	Test	U (MeV)	r_u (fm)	a_u (fm)	W (MeV)	r_w (fm)	a_w (fm)	χ^2/N	Δ/N
^{28}Si + ^{4}He	63	26.5	χ^2	75.62	1.13	0.47	8.39	1.13	0.47	1474	(2668)
	"	"	Δ	75.68	"	"	9.38	"	"	(3047)	1192
^{40}Ca + ^{4}He	62	24.15	χ^2	64.60	1.16	0.52	6.25	1.16	0.52	1626	(3187)
	"	"	Δ	64.68	1.16	0.52	9.09	"	"	(11 306)	737
^{28}Si + ^{16}O	92	54.69	χ^2	148.87	1.189	0.47	10.54	1.189	0.47	20.65	(45.54)
	"	"	Δ	148.91	"	"	12.56	"	"	(82.32)	23.50
^{208}Pb + ^{4}He	34	26.0	χ^2	25.06	1.22	0.55	6.69	1.22	0.55	7.6	(7.3)
	"	"	Δ	25.31	1.22	0.55	6.58	1.22	0.55	(7.3)	7.6

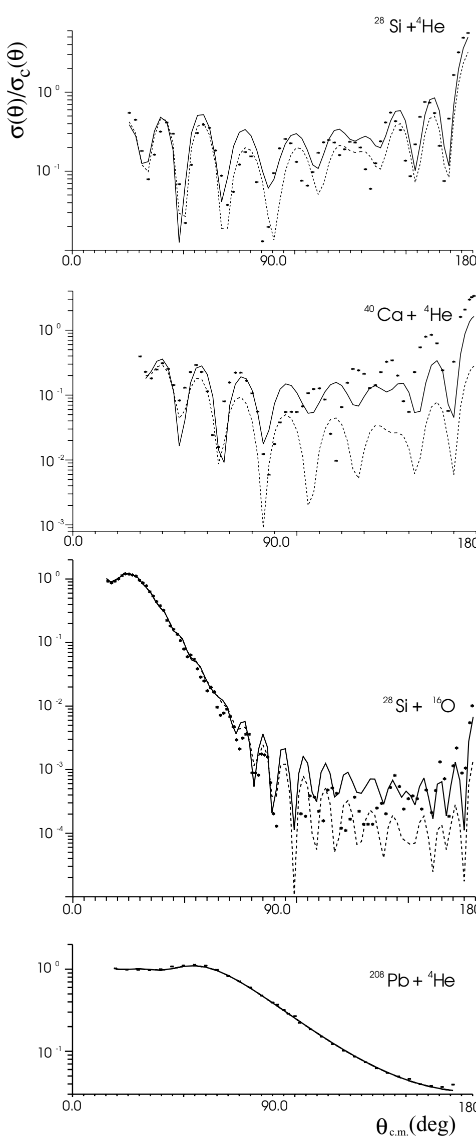

FIG. 3. The elastic angular distributions calculated for the parameters of minima of χ^2 (solid curves) and Δ (dashed curves) test functions listed in Table I for a set of four experimental elastic scattering data.

Table I. A detailed study of the χ^2 and Δ surfaces shows that, apart from the vicinities of deep minima, the first surface is very "wavy" and has many local minima where the search based on the gradient analysis stops, whereas the Δ function surface is very smooth and the search usually reaches the nearest deep minimum. When the χ^2 test is used, it is necessary to scan its surface first, and next to perform the search within the deep minima. By adding more free parameters to the OM, we can slightly improve the quality of the fits, but the preceding differences still persist.

IV. DISCUSSION

The goodness-of-fit function used in the automatic search for the best parameters of any theoretical model used to fit sets of experimental data must have an absolute minimum for those model parameters that reproduce perfectly the experimental points, and it must have a minimum for the set of those model parameters that describe the experimental data only with certain accuracy. Moreover, it is clear that a good test function should be symmetrical around the minimum, as it is only in this case that the predicted values would be symmetrically distributed around the experimental values. Which function we select as a test function while performing the automatic searches for the best set of the studied model parameters is a matter of convention, but we must keep in mind the fact that various functions might operate in a different way, and the computer will choose a set of parameters that is not always the best. The test function must also give a statistical measure-of-fit quality, and it is clear that the χ^2 function can guarantee this.

Here I present a very simple example of the analysis of elastic differential cross sections by means of a very simple phenomenological four-parameter OM. The elastic differential cross section is the simplest nuclear reaction observed, but of a very specific type. This differential cross section is a superposition of two phenomena, namely nuclear diffraction and nuclear refraction [6]. The origins of these phenomena and their mechanisms are quite different. The diffraction picture forms beam particles that pass by the nucleus and have no contact with it (have no contact with the nuclear forces). The refraction picture forms particles that pass through the

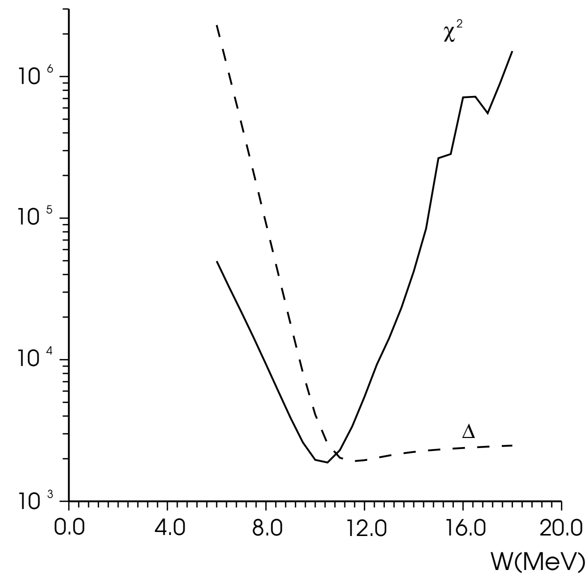

FIG. 4. The profiles and positions of the deepest minima of χ^2 (solid curve) and Δ (dashed curve) test functions in the W direction for the ^{40}Ca + ^{4}He case.

nucleus, are in contact with it, and are affected by nuclear forces. Diffraction, being a purely wave effect, can be correctly described by the "incomplete" Coulomb scattering amplitude. The refraction mechanism is much more complicated and can be described only approximately by means of complex nuclear potential of the OM. The diffractive cross section, which is very strong, dominates at forward angles, whereas the refractive one, which sometimes is only a fraction of a percentage of the whole elasic effect, rises above the diffractive tail at backward angles. If we fit the whole elastic angular distribution with the OM, the automatic search routine with the Δ test function will easily find a set of parameters that reproduce the diffractive forward-angle part of the angular distribution, and, because of its high asymmetry (see Fig. 4), will pay much less attention to its backward-angle part. The Δ test function will then select parameters giving $\sigma_T \ll \sigma_E$ for the refractive cross section. In a real situation, the asymmetry of the Δ function is even higher because of higher statistical errors at backward angles (compare Figs. 4 and 1). This is a common situation when the elastic differential cross section is fit with the OM by use of the Δ test function. The whole elastic scattering angular distributions of strongly absorbed particles and heavy ions cannot be reproduced perfectly by the simple OM. To get better fits to the backward-angle parts of the cross sections, we must add more free potential parameters to the OM or include some other effects, like narrow resonances. First, however, we must determine the set of pure OM parameters that give the best possible fit to the data. By adding resonances to the elastic scattering cross-section analysis we in fact add another effect of yet another different mechanism and origin (surface). In the simple analyses just presented, the χ^2 test is definitely better in the first three cases. In the case of ^{208}Pb + ^{4}He, which is almost pure diffraction [6], of course both functions give the same results.

A similar situation might exist when any other experimental data are fit with a model that is unable to reproduce them perfectly.

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