THE ACCURACY OF HEAVY-ION OPTICAL MODEL CALCULATIONS

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Heavy ion elastic scattering calculations lead to numerical difficulties in the regions of energies and angles where the cross sections are small. Two different approximate methods have been investigated in the case of $^{20}Ne + ^{24}Mg$ scattering at $E_{LAB} = 100$ MeV. The emerging errors of calculations are traced in detail. It is shown, that the optical model calculations are critically sensitive to some details which are arbitrarily assumed in commonly used approximate methods. The obtained results allow to perform similar calculations with controlled accuracy and some ambiguities of optical model potentials can be removed.

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1. Introduction

Well defined numerical accuracy of the optical model calculations appears as a trivial, but in some sense crucial problem in all heavy ion elastic scattering analyses. Numerical methods commonly used for solving the Schödinger equation contain some approximations. Due to these approximations the angular distributions are calculated with some errors depending on the magnitude of angular momentum and on the angular region of scattering. The resulting accuracy is limited by the available computer time and is determined for a given numerical method by values of some parameters of the program. The values are set automatically by the code or should be chosen arbitrarily by the user. The errors resulting from this procedure can be found by comparing the results obtained by means of an optical model code with angular distributions calculated with a much higher accuracy. Two such reference methods were recently proposed by Doering et al. [1] and Dymarz and Małecki [2].

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The aim of this paper is to check errors of the optical model code when the Fox–Goodwin method [3] is applied for heavy ion elastic scattering in the region of masses $A \leqslant 40$ and energies of about 1 MeV per nucleon.

It is well known that the analysis of data of the elastic scattering of complex nuclei yields optical model potentials which are ambiguous at the nuclear surface and meaningless in the nuclear interior. The ambiguity disappears only around the "sensitive radius" distance [4], but does not favour any of the equivalent potentials [5]. It was also found that the crossing point at the sensitive radius follows as a consequence of the conservation of the volume integral at the surface of the real part of optical potential [6].

The physical properties of the potential like strong absorption, surface transparency [7] or l-dependent absorption [8] are displayed best at the backward region of elastic scatter-

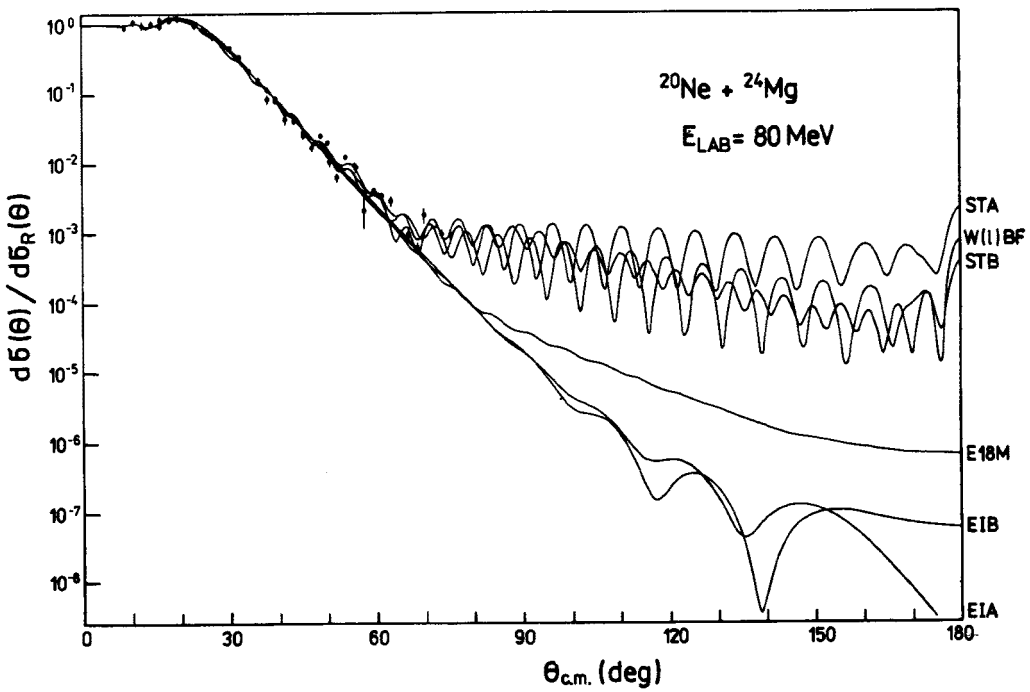


Fig. 1. Equivalent fits to forward data of elastic scattering $^{20}Ne + ^{24}Mg$ with strong absorptive potentials EIA, EIB and E18M, surface transparent potentials STA and STB and potential with l-dependent absorption $W(l)$BF

ing angular distribution. In the case of $^{20}Ne + ^{24}Mg$ elastic scattering at 80 MeV [9] one can see that most of the equivalent potentials fitting forward data could be ruled out by the measurement of the backward data (see Fig. 1).

This example makes it clear that precise optical model calculations are necessary if ambiguities are to be investigated. Besides the backward data, the results of fusion $^{20}Ne + ^{24}Mg$ are desirable as a complementary bound for the optical model potentials [10].

2. Sources of errors

For central forces the elastic scattering cross section is given by the following partial wave expansion:

$$d\sigma(\theta) \sim \left| f_{\text{coul}}(\theta) + \frac{1}{2ik} \sum_{L=0}^{\infty} (2L+1)\,(S_L - 1) e^{2i\sigma_L} P_L(\cos\theta) \right|^2 . \tag{1}$$

The most evident, error of this expansion, ε_L, is caused by truncation of the partial wave sum after some $L_{\max}$ (see Fig. 2). The optimum value of $L_{\max}$ can be found from the limiting conditions assumed for the matrix element S_L. In all calculations presented in this paper we have fixed $L_{\max}$ so large that Im S_L was equal to zero in the CDC CYBER 72, 64 bit word

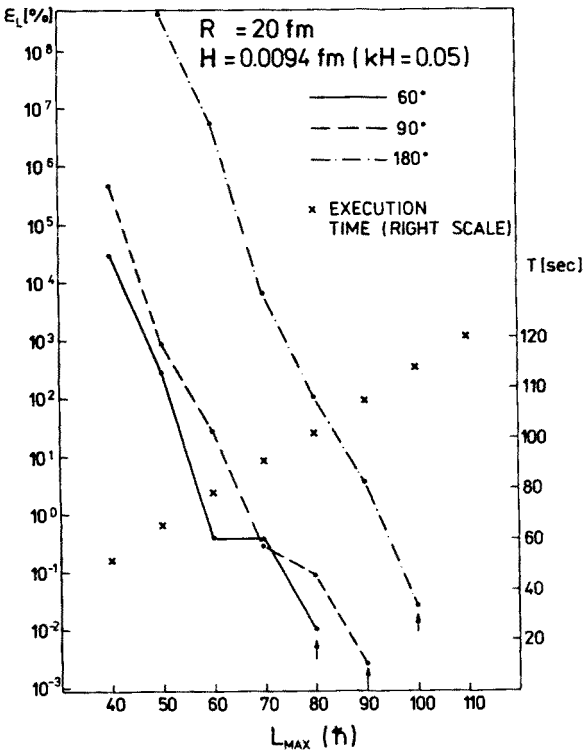


Fig. 2. Dependence of the cross section errors at $\theta_{CM} = 60°$, 90° and 180° on truncation value $L_{\max}$ of the partial wave expansion (1) and the dependence of the computer time consumption

representation. The resulting accuracy is indicated by arrows in Fig. 2. The additional scale in Fig. 2 represents the central processor execution time, necessary to perform calculation with a given $L_{\max}$ value. As one can see it is simply proportional to $L_{\max}$.

Another computing error arises from the wrong setting of the matching radius R_M. This is a distance where the internal solution of the Schrödinger equation should be matched

with the combination of the Coulomb regular and irregular functions. Melkanoff et al. [11] have derived the approximate formula for the corresponding error of scattering matrix for the Woods–Saxon shape of the potential:

$$\varepsilon_M \sim \frac{Vka}{E} \exp\left[-\left(\frac{R_M - R}{a}\right)\right], \tag{2}$$

where V, R and a are the depth, radius and diffuseness of the potential well, and E and k are the energy and wave number of the projectile, respectively.

The third error ε_T of the S matrix is due to the fourth order termination of the Taylor expansion of the wave function in the region of r close to zero.

$$\varepsilon_T \sim H^4 \int_0^{R_M} \psi \frac{d^6\psi}{dr^6}\, dr. \tag{3}$$

The round-off error ε_R results from the use of a computer word of some final lenght (e.g. 64 bits for the CYBER 72, in single precision). The magnitude of this error depends on H, R_M in the following way:

$$\varepsilon_R \sim \frac{1}{H^2} \int_0^{R_M} \psi^2 dr. \tag{4}$$

Inspection of Fig. 2 and formulas (2), (3), (4) shows that the accuracy of the optical model calculations depends mainly on the matching radius R_M and the integration step size H. The aim of our investigation was to find a domain in the $R_M - H$ space for which the error of $\sigma(\theta)$ is stable and reasonably small compared with experimental errors and the computer time consumption. Due to its monotonic dependence, error ε_L can be easily avoided or limited to the desired magnitude by using a large enough L_{max} value.

Despite its importance we do not deal here with the Coulomb part of the optical model calculation. For all our tests we have used the Coulomb subroutine RCWFN [12] well examined elsewhere, which is believed to cause negligible errors by itself. We also used the uniformly charged sphere as a simplified model of the charge distribution. Its radius was assumed to be $r_c = 1.0$. Incidentally, it is not critical for the optical model calculations [13]. It was not desirable in our case to introduce a more realistic charge distribution [14], so to save computer time it was not included here.

3. Reference calculations

The errors described by formulas (2), (3), (4) are unnormalized and their simultaneous influence on the resulting error must be calculated practically in absolute values. Then it is necessary to compare the results of an investigated code with highly accurate results. One of the possible ways to get the reference results is based on the Born approximation [15]. This was successfully applied for the $^3H + {}^{60}Ni$ system by Doering et al. [1] at incident

energy 70 MeV. However, even the second order Born approximation fails for low l-values and higher orders are suppressed by rapidly increasing computer time consumption.

We have decided to explore another possibility based on the Dymarz–Małecki method [2]. In contrast to the standard methods, they used the wave functions which are exact solutions of the approximating potential, rather than approximate solutions of the exact potential. They applied a sum of a large number of rectangular wells with the envelope following the approximated potential. This allows to get an exact solution (combination of spherical Hankel functions) of radial Schrödinger equation with approximated potential.

The method was found to be very suitable for the heavy ion problem, where rather large k wave numbers are present. This advantage comes from the fact that the radial dependence of the potential is much smoother then that of the wave function. This is revealed by the rapid convergence of the solutions even for a relatively small number of approximating rectangular wells. The stable values of $\sigma(\theta)$ for all angles θ are available begining from about 1500 divisions and any further splitting does not change the results significantly up to 5000 divisions. The number of required divisions in numerical integration appears also practically independent of k, unlike in methods approximating the wave function.

Basing on the above we assigned to the values $\sigma_{SQ}(\theta)$ errors equal to zero according to formula (5). Both the SQUAR code [16], based on the Dymarz–Małecki method, and the tested one, OPTY [17], contain the same Coulomb subroutines, which suppress any additional relative discrepancies.

4. *Results*

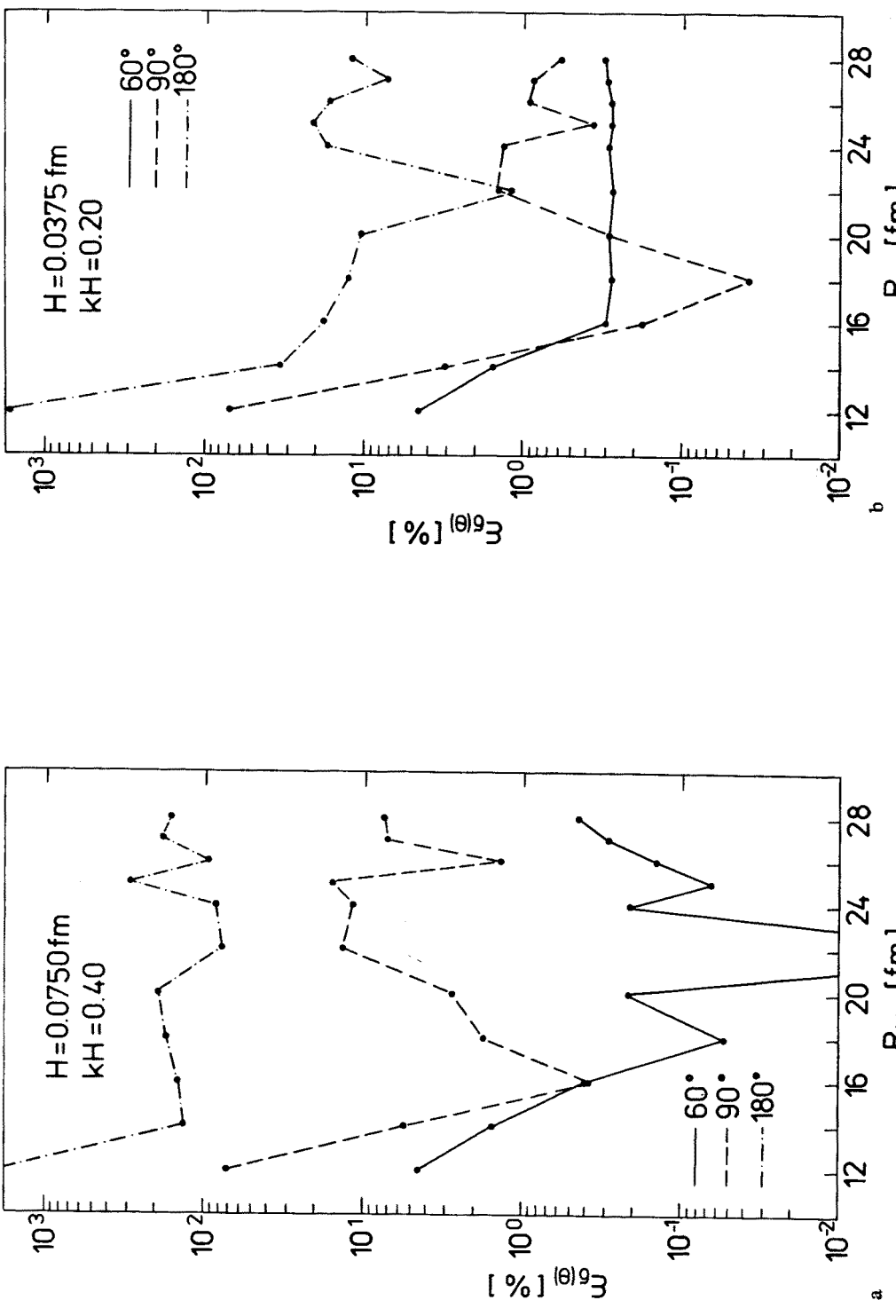
As ε_M, ε_T and ε_R have the opposite dependence on R_M and H, it was necessary to make a two-dimensional map of errors. Our research was performed on $\sigma(\theta)$ rather then on S_L because this is the experimentally measured value. However, it can be expected that the follwing results are still valid for the cases where for instance the S_L matrix elements are to be modified by the Regge pole terms [18] and accuracy is most significant. The error is defined by:

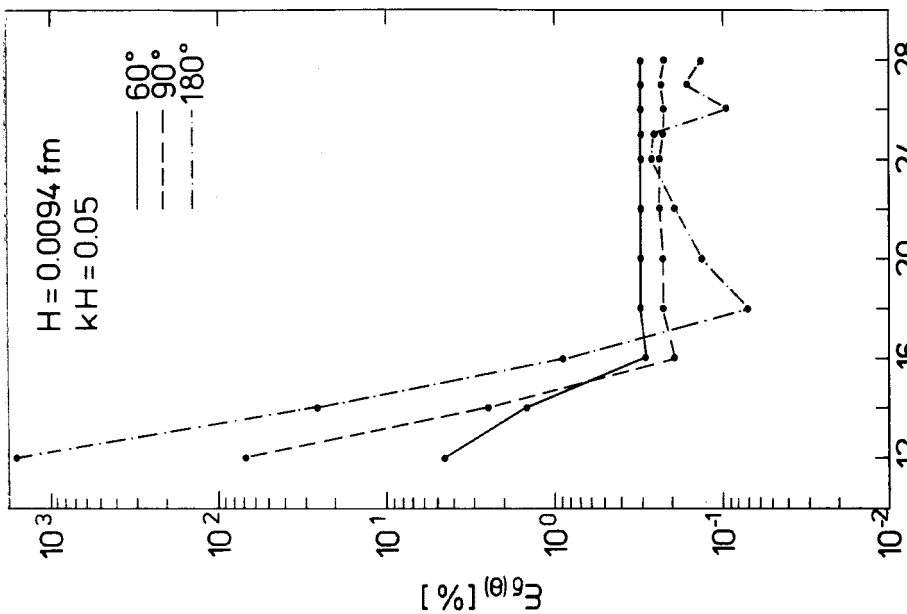
$$\varepsilon_{\sigma(\theta)} = \frac{|\sigma_{OPT}(\theta) - \sigma_{SQ}(\theta)|}{\sigma_{SQ}(\theta)} \times 100\%. \tag{5}$$

The $\sigma_{SQ}(\theta)$ values of the cross sections were obtained with the SQUAR code described in the previous section. $\sigma_{OPT}(\theta)$ were calculated with the investigated optical model code.

Our tests were performed over the step size of integration H = 0.0094, 0.0187, 0.0375, 0.0750 fm (kr = 0.05, 0.1, 02, 0.4) and for matching radius R_M = 12, 14, 16, 18, 20, 22, 24, 25, 26, 27, 28 fm. These ranges implied that the number of steps varied from 160 to 3000. All calculations concerned $^{20}Ne + ^{24}Mg$ elastic scattering at 100 MeV and used one of the best fit potentials [9]. According to R_M 80 to 150 partial waves were incorporated.

We did not get any smooth error function of $\sigma(\theta)$ because of the cancellation effects in partial wave sums, but our results illustrate its overall behaviour. On Figs 3a, b, c, d the errors of $\sigma(\theta)$ for θ_{CM} = 60°, 90° and 180° are plotted as a function of the matching radius


H=0.0750fm
kH=0.40
60°
90°
180°
$\varepsilon_{\sigma(\theta)}$ [%]
R_M [fm]
a
H=0.0375 fm
kH=0.20
60°
90°
180°
$\varepsilon_{\sigma(\theta)}$ [%]
R_M [fm]
b



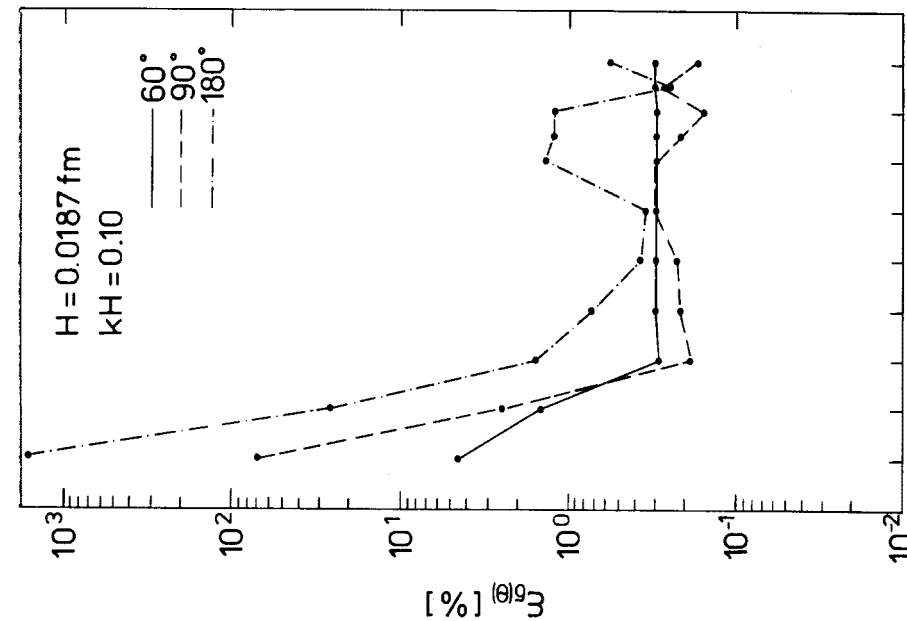
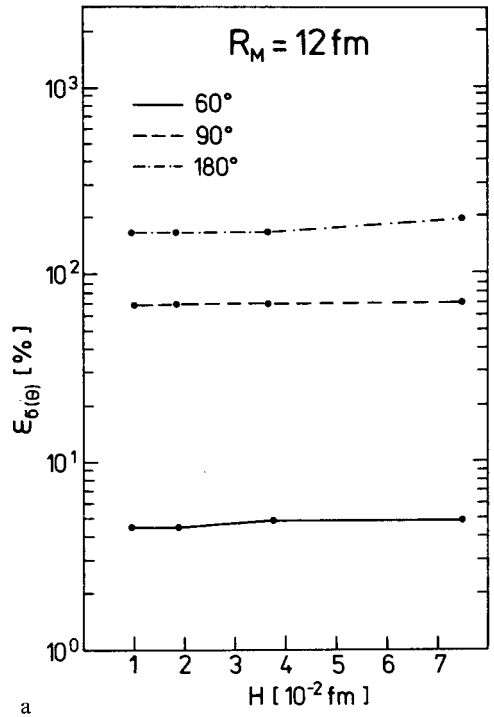
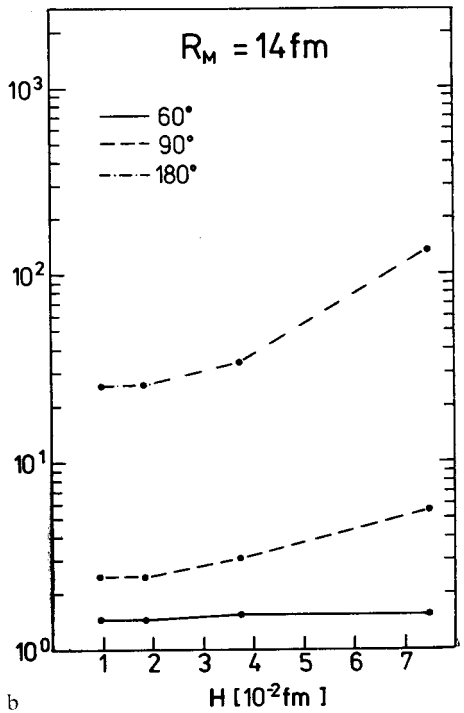
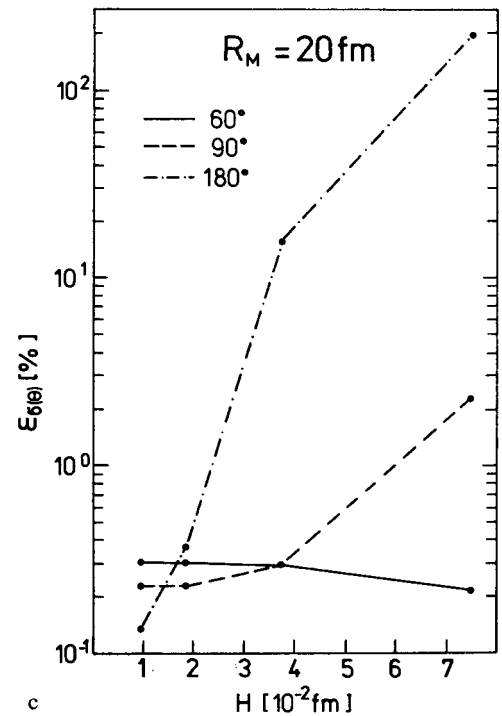
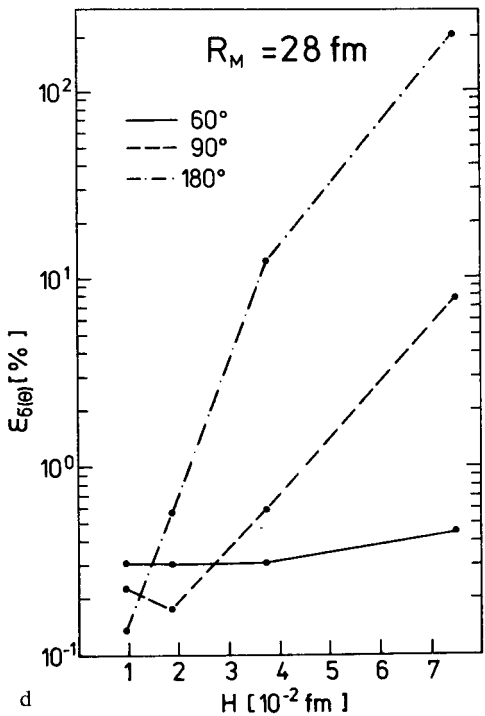


Fig 3a, b, c, d. The errors of the cross section calculations at $\theta_{CM} = 60°$, 90° and 180° as a function of matching radius R_M for fixed step sizes of integration H









Figs 4a, b, c, d. The errors of the cross section calculations at $\theta_{CM} = 60°$, 90° and 180° against the step size H for the constant values of matching radius R_M

R_M. Each plot concerns the fixed step size H. Figs 4a, b, c, d show the same errors against the step size H when the matching radius R_M is held constant.

It can be seen in all of Figs 3 that the matching radius error dependence of formula (2) is well pronounced by the exponential decrease at small R_M. The strong dependence of the error stabilizes from about 18 fm and becomes oscillating for some larger R_M values. It was found that for reasonably small steps the error is insensitive to R_M for the forward angles ($\theta_{CM} = 60^\circ$) and for $R_M \geqslant 16$ fm it is less than 0.3%. Figs 4a and 4b illustrate the observation that for too small matching radii errors are almost constant when H is varied, according to H independent formula (2). The magnitude of this errors damps completely other possible contributions. This is not the case in Figs 4c and 4d, where it rises strongly with increasing H-step like truncation error from formula (3). Its slope does not follow the H^4 dependence, except for the error at $\theta_{CM} = 180^\circ$.

5. *Conclusions*

We have checked the sensitivity of optical model calculations of $\sigma(\theta)$ to the matching radius and to the step size in the numerical integration of the Schrödinger equation. It is shown that extreme care should be devoted to the far backward scattering cross sections. The forward data, especially those of $\theta_{CM} < 60^\circ$, can be fitted with insignificant errors whereas at backward region precise fits are imposible. Let us emphasize that it is necessary to verify the numerical accuracy of calculations when a new heavy ion system is considered or an unknown code applied. It was found that for $^{20}Ne + ^{24}Mg$ at 100 MeV the optimum values of R_M and H are about 20 fm and 0.02 fm, respectively. At this matching radius the nuclear potentials reach 10^{-9} of their central strength, thus stressing the great importance of the far tailing region of the nuclear potential [6]. The 10^{-3} rule, commonly used for light projectiles, now fails completely ($R_M = 12$ fm), producing enormous errors. It seems that the Hodgson rule [19] for the step size is still valid and predicts that each unit of kr should be divided into ten steps approximately. In our case $kr = 0.1$ yields $H = 0.019$.

In general, when the true value of the optical model cross section is unknown, the optimum values of R_M and H can be chosen according to the behaviour of the errors of $\sigma(\theta)$. So $\theta = 180^\circ$ is recommended for these tests as the most sensitive region. Then, for the fixed R_M two calculations should be performed with H steps ranging over one decade. Next, if the two values of $\sigma(\theta)$ differ approximately by four orders of magnitude it can be claimed that this R_M is not too small. The weaker H-dependence of $\sigma(180^\circ)$ (when a 64 bit word is used) should be interpreted so that R_M must be increased. The above recipe can be invalid for calculations performed with a shorter computer word. The round-off error, according to formula (4) can complicate the situation, producing a relatively deep minimum in the $R_M - H$ space.

We still believe that although backward angles are connected with the biggest experimental and numerical difficulties, they contain the most conclusive information on heavy ion interaction available from elastic scattering.

I wish to thank Professor K. Grotowski for stimulating discussions.

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