# The Numerical Accuracy of ${ }^{3} \mathrm{He}$ Optical-Model Calculations at 70 MeV * 

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#### Abstract

Small differential cross sections, such as those measured at back angles for 70 MeV ${ }^{3} \mathrm{He}$ elastic scattering (typically below $10^{-4} \mathrm{mb} / \mathrm{sr}$ past $130^{\circ}$ ), are difficult to calculate accurately when they result from considerable cancellation in the partial-wave sum. The codes GENOA, GIBELUMP, SNOOPY3, and DWUCK differ by as much as $2 \frac{1}{2}$ orders of magnitude on $\sigma(\theta)$ for an optical-model potential describing ${ }^{60} \mathrm{Ni}\left({ }^{3} \mathrm{He}\right.$, $\left.{ }^{3} \mathrm{He}\right)^{60} \mathrm{Ni}$ scattering at 71 MeV . This calculation is repeated, with a modified version of GIBELUMP, for wide ranges of the parameters affecting numerical accuracy. A study of errors in scattering matrix elements and cross sections, as functions of these parameters, reveals that criteria commonly used to determine the matching radius and number of partial waves employed in optical-model calculations yield insufficient values in this case.


## 1. Introduction

There is increasing evidence that the well known ambiguities in optical-model potentials for complex projectiles may be at least partially resolved through analyses including large angle elastic scattering data [1-5], especially at relatively high bombarding energies. In particular, S. M. Smith and D. A. Goldberg [1] have noted a sensitivity of back-angle deuteron, helion, and alpha-particle elastic scattering to real well depth at incident energies above 60 MeV . The characteristic feature of such data is a monotonic fall (with increasing angle) beyond the diffraction region. Such behavior is illustrated in Fig. 1, which presents $70 \mathrm{MeV}^{3} \mathrm{He}$ elastic angular distributions, taken from targets of ${ }^{50} \mathrm{Ti}$ and ${ }^{51} \mathrm{~V}$ with the MSU Sector-Focused Cyclotron [2]. Similar data have been obtained by C. B. Fulmer and J. C. Hafele. They also stress the importance of the small, back-angle cross sections for suppressing ambiguities in the ${ }^{3} \mathrm{He}$ optical-model parameters [3].

Unfortunately, we find that unusual care is required for the accurate calculation of such small cross sections, since they result from a great deal of cancellation

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Fig. 1. $70 \mathrm{MeV}^{3} \mathrm{He}$ elastic scattering data taken from targets of ${ }^{50} \mathrm{Ti}$, and ${ }^{51} \mathrm{~V}$.
in the partial-wave sum. The associated loss of significance can lead to difficulties of the type indicated by Fig. 2. This is a comparison of ${ }^{60} \mathrm{Ni}\left({ }^{3} \mathrm{He},{ }^{3} \mathrm{He}\right){ }^{60} \mathrm{Ni}$ scattering at 71 MeV , as calculated with the optical-model codes GENOA [6], GIBELUMP [7], and SNOOPY 3 [8], and the DWBA code, DWUCK [9]. All programs used the following potential (including the parameters with which we intended to start searches on the data of Fig. 1):

$$
\begin{equation*}
U(r)=U_{c}-V_{R} f\left(x_{R}\right)+i 4 W_{D} \frac{d}{d x_{I}} f\left(x_{I}\right) \tag{1}
\end{equation*}
$$

where

$$
\begin{aligned}
U_{c} & =\frac{Z Z^{\prime} e^{2}}{2 R_{c}}\left(3-\frac{r^{2}}{R_{c}^{2}}\right), \quad \text { for } r \leqslant R_{c} \\
U_{c} & =\frac{Z Z^{\prime} e^{2}}{r}, \quad \text { for } r \geqslant R_{c} \\
R_{c} & =r_{c} A^{1 / 3} \\
f(x) & =\left(1+e^{x}\right)^{-1} \\
x_{R} & =\frac{r-r_{R} A^{1 / 3}}{a_{R}},
\end{aligned}
$$

and

$$
x_{I}=\frac{r-r_{I} A^{1 / 3}}{a_{I}}
$$

with $V_{R}=126.5 \mathrm{MeV}, r_{R}=1.12 \mathrm{~F}, a_{R}=0.837 \mathrm{~F}, W_{D}=20.4 \mathrm{MeV}, r_{I}=1.26 \mathrm{~F}$, $a_{I}=0.841 \mathrm{~F}$, and $r_{c}=1.3 \mathrm{~F}$ [10]. At forward angles, where the cross sections are large, the four codes agree quite well. However, at back angles, the cross sections are small, and there are discrepancies of as much as $2 \frac{1}{2}$ orders of magnitude. Similar comparisons for 30 MeV helion and 50 MeV proton elastic scattering (with typical parameters) show less dramatic and negligible differences, respectively,


Fig. 2. Comparison of elastic scattering calculated with four codes from the same potential. The reference lines are from a more accurate calculation with a modified version of GIBELUMP, which employed the optimum numerical accuracy parameters defined in the text.
the magnitude of the percentage disagreement being, in general, inversely related to the size of the cross section. When the ratio to Rutherford scattering is above $10^{-2}$, we find little problem, but when it drops below $10^{-4}$, the calculation appears beyond the scope of many codes. This paper investigates a particular case, which falls into the latter category, back-angle scattering in the aforementioned $71 \mathrm{MeV}{ }^{60} \mathrm{Ni}\left({ }^{3} \mathrm{He},{ }^{3} \mathrm{He}\right)^{60} \mathrm{Ni}$ problem.

## II. Sources of Error in Optical-Model Calculations

Neglecting spin-dependent forces, the partial-wave expansion of the elastic scattering amplitude may be written [11]:

$$
\begin{equation*}
f(k, \theta)=f_{c}(k, \theta)+\frac{1}{2 i k} \sum_{\ell=0}^{\infty}(2 \ell+1)\left(S_{\ell}-1\right) e^{2 i \sigma_{c}} P_{t}(\cos \theta) . \tag{2}
\end{equation*}
$$

The most obvious source of error is the necessity to truncate the partial-wave sum after some $\ell=L_{\text {max }}$. There is also the aforementioned loss of significance due to cancellation in the sum. We may compensate for the loss of significance by calculating the individual terms more accurately. The Legendre polynomials $\left(P_{t}\right)$ are easily evaluated from their well known recurrence relations, and expressions for $\ell=0$ and 1 [12]. The Coulomb scattering amplitude $\left(f_{c}\right)$ is a relatively simple function of the zero-order Coulomb phase shift ( $\sigma_{0}$ ), which may be obtained along with the other $\sigma_{l}$ 's by downward recursion from an asymptotic expansion for $\sigma_{L}$, with $\ell=L$ chosen large enough for any desired accuracy [13]. The real difficulties arise in calculating the scattering matrix elements ( $S_{\ell}$ ). The optical-model codes accomplish this by matching "internal" and "external" solutions of the radial Schroedinger equation at a radius $r=R_{M}$. The internal solution is generated by numerically integrating the Schroedinger equation from the origin to the matching radius. The external solution is taken to be a linear combination of regular and irregular Coulomb functions. Thus, several potential sources of error are immediately evident.
If $R_{M}$ is not chosen large enough to make the effects of the nuclear potential negligible, the Coulomb wave function will be a poor representation of the exact solution at that radius. Melkanoff, Raynal, and Sawada have derived [14] an approximate form of this error in the scattering matrix for the case of a WoodsSaxon potential:

$$
\begin{equation*}
\epsilon_{F} \propto \frac{V k a}{E} \exp \left[-\left(\frac{R_{M}-R}{a}\right)\right], \tag{3}
\end{equation*}
$$

where $V, R$, and $a$ are the depth, radius, and diffuseness, respectively, of the WoodsSaxon well, and $E$ and $k$ are the energy and wave number of the incident particle. They also give the following expressions for truncation $\left(\epsilon_{T}\right)$ and round-off $\left(\epsilon_{R}\right)$ errors in $S_{\ell}$, which accumulate during the numerical integration:

$$
\begin{equation*}
\epsilon_{T} \propto H^{4} \int_{0}^{R_{M}} \psi \frac{d^{6} \psi}{d r^{6}} d r \tag{4}
\end{equation*}
$$

and

$$
\begin{equation*}
\epsilon_{R} \propto H^{-2} \int_{0}^{R_{M}} \psi^{2} d r, \tag{5}
\end{equation*}
$$

where $H$ is the step size and $\psi$ is the radial wave function. Equations (4) and (5) are valid for the fourth-order Cowell [14] (also known as Fox-Goodwin [15]) method, which is widely used for integrating second-order differential equations without a first-order term, such as the radial Schroedinger equation with a local opticalmodel potential. The order of the integration method refers to the finite number of terms retained in a Taylor series which represents the solution locally. The neglect of higher-order terms yields the truncation crror. The round-off error results from the use of a limited number of digits in the calculation. Equations (4) and (5) indicate that both of these errors may grow with $R_{M}$. Thus, it may be possible to select too large, as well as too small, a matching radius.

The same problem is apparent for integration step size. If $H$ is very small, the truncation error will be small, but the round-off error, large, and vice versa. Hopefully, some domain of $H$ (and $R_{M}$ ) will always exist for which these errors in the scattering matrix elements remain suitably bounded.

The scattering matrix also receives errors from the Coulomb wave functions, which may be evaluated by a variety of techniques, each fraught with unique difficulties. For relatively small values of the Coulomb parameter $\eta\left(=\mu Z Z^{\prime} e^{2} / k \hbar^{2}\right)$, and large values of $\rho(=k r)$, the Coulomb functions are commonly calculated with recursion relations and asymptotic expansions [16]. Except for a normalization factor, the regular Coulomb functions ( $F_{\ell}$ ) may be obtained by downward recursion from $F_{\mathscr{L}+1}=0$ and $F_{\mathscr{L}}=\delta$, an arbitrary "small" number. As in the case of Coulomb phase shifts, a particular $\ell=\mathscr{L}$ is chosen, which determines the accuracy at lower $\ell$ 's. The normalization may be found by requiring the Wronskian of the zero-order Coulomb functions to equal 1 . One of the required derivatives, $F_{0}{ }^{\prime}$, is simply related to $F_{0}$ and $F_{1}$. Unfortunately, the asymptotic series for the zero-order irregular function and its derivative are only semiconvergent. If summing until the series begin to diverge does not give the desired accuracy, they may be summed at a larger radius ( $\mathscr{R}$ ), where the initial convergence is more rapid. The resulting values may then be used to start a numerical integration of the Schroedinger equation, containing only the Coulomb potential, inward to the matching radius. At this point, upward recursion will generate the irregular Coulomb functions ( $G_{\ell}$ ) for the higher $\ell$ 's. Upward recursion preserves significance for the irregular functions, since they generally grow in magnitude with increasing $\ell$, opposite to the behavior of the regular functions.

We have mentioned the major sources of error in a typical optical-model calculation of an elastic scattering amplitude. The errors in the partial-wave amplitudes each have associated "numerical accuracy parameters" (e.g., $R_{M}$ ), which control particular approximations. We seek values of these parameters which yield very accurate individual amplitudes, a few significant figures of which will survive the extreme cancellation in the partial-wave sum for small cross sections.

## III. Errors in the Scattering Matrix

The code GIBELUMP has been modified so that the aforementioned numerical accuracy parameters may be specified externally and varied over wide ranges. If we simplify matters by always evaluating the asymptotic expansions of the Coulomb functions at the matching radius (i.e., setting $\mathscr{R}=R_{M}$ ), we are left with four such parameters: $L, \mathscr{L}, R_{M}$, and $H$. The first pair is rather easy to set, since the associated errors diminish as $L$ and $\mathscr{L}$ become larger. Therefore, we merely need to increase these parameters until the scattering amplitudes remain constant to the number of significant figures desired. However, the matching radius and integration step size cannot be dealt with in such an elementary manner. As we have seen, there are errors coupled to $R_{M}$ and $H$ which have opposite dependences on these parameters. Thus, the net error in each partial-wave amplitude may be a complicated function of the matching radius and integration step size. To facilitate selection of $R_{M}$ and $H$ for our ${ }^{3} \mathrm{He}$ elastic scattering calculation, we have investigated this function (for several values of $\ell$ ) at matching radii between 10 F and 30 F and step sizes from 0.0075 F to 0.2 F . Since these two parameters enter a partial-wave amplitude only through $S_{\ell}$, it is sufficient to consider errors in the scattering matrix alone. Also, since the Coulomb parameter is small ( $\eta<2$ ) for our case, we do not expect these errors to be significantly affected by the calculation of Ricatti-Bessel [17], rather than Coulomb, functions (i.e., setting $\eta=0$ ). Thus, we have omitted the Coulomb potential from the computations discussed in this section. This enables us to alternatively calculate $S_{\ell}$ 's from second-order Born approximation solutions to the coupled integral equations for the phase shifts [18]. Such calculations were performed with the code PWBA2 [19]. The scattering matrix elements in Table I were obtained with PWBA2 and the modified GIBELUMP (with $H=0.0125 \mathrm{~F}, R_{M}=25.0 \mathrm{~F}, \mathscr{L}=100$, and $L=101$ ). Both codes employed the previously listed ${ }^{3} \mathrm{He}-{ }^{60} \mathrm{Ni}$ potential (except for the Coulomb term) at an incident ${ }^{3} \mathrm{He}$ energy of 71 MeV . Since PWBA2 and GIBELUMP use entirely different methods of arriving at the $S_{\iota}$ 's, the extent to which they agree indicates a lower bound on the accuracy of each. As the partialwave number increases, the Born series converges more rapidly (for suitable potentials), and it appears that PWBA2 is accurate to $\gtrsim 8$ decimal places for $\ell \gtrsim 40$. Thus, we may define errors in the scattering matrix elements calculated with the modified GIBELUMP (which will be meaningful if larger than about $10^{-8}$ for $\ell \geq 40$ ) by

$$
\operatorname{Re} \epsilon_{\ell}=\left|\operatorname{Re} S_{\ell}^{\mathrm{PWBA} 2}-\operatorname{Re} S_{\ell}^{\mathrm{GIBELUMP}}\right|
$$

and

$$
\operatorname{Im} \epsilon_{\ell}=\left|\operatorname{Im} S_{\ell}^{\mathrm{PWBA} 2}-\operatorname{Im} S_{\ell}^{\mathrm{GIBELUMP}}\right|
$$

Figure 3 shows the dependence of these errors on matching radius for $H=0.015 \mathrm{~F}$ and $\ell=40,50$, and 60 . The scattering matrix elements are extremely close to unity, and the corresponding errors almost constant, until $R_{M}$ reaches the classical impact parameter $R_{\ell}=\ell / k\left(k \approx 3 F^{-1}\right)$ for each partial wave. Farther out we observe an exponential decrease, as predicted by Eq. (3) for the finite matching radius error. The region of minimum observable error extends from about 22 F to 25 F , beyond which an exponentially increasing error becomes measurable. This confirms our previous speculation that $R_{M}$ can be chosen too large.


Fig. 3. Dependence of errors in scattering matrix elements on matching radius for a 0.015 integration step size.

There appear to be two major sources of error contributing to the $\epsilon_{\ell}$ 's. One dominates at small matching radii and decreases exponentially with $R_{M}$, eventually being overtaken (somewhere outside 20 F ) by the other, which increases exponentially. Since GIBELUMP employs a fourth-order Cowell numerical integration algorithm, Eqs. (4) and (5) may be used to interpret the dependence of the scattering matrix errors on integration step size (for fixed matching radii). With $R_{M}=15 \mathrm{~F}$, Fig. 4 indicates that the $\epsilon_{\epsilon}$ 's are independent of step size. Thus, the major source of error for $R_{M} \lesssim 20 \mathrm{~F}$ does not behave like truncation (Eq. (4)) or round-off (Eq. (5)). However, its behavior as a function of $H$ (as well as $R_{M}$ ) is consistent with Eq. (3), which describes the error due to finite matching radius. For

TABLE I
Comparison of Scattering Matrix Elements Calculated with the Modified GIBELUMP (OpticalModel Code) and PWBA2 (Second-Order Born Approximation Code) ${ }^{a}$

|  | Real $S_{\ell}$ |  | Imaginary $S_{\ell}$ |  |
| :---: | :---: | :---: | :---: | :---: |
| $\ell$ | GIBELUMP | PWBA2 | GIBELUMP | PWBA2 |
| 20 | 0.12941772 | 0.00101740 | 0.09446676 | 0.28783675 |
| 21 | 0.25494459 | 0.20751226 | 0.15728529 | 0.27749207 |
| 22 | 0.40959841 | 0.39774516 | 0.18916798 | 0.25166682 |
| 23 | 0.55919313 | 0.55834389 | 0.18627662 | 0.21455524 |
| 24 | 0.68339913 | 0.68449549 | 0.16157908 | 0.17316819 |
| 25 | 0.77761587 | 0.77846355 | 0.12928026 | 0.13372584 |
| 30 | 0.96526366 | 0.96527341 | 0.02580755 | 0.02583216 |
| 35 | 0.99466337 | 0.9946340 | 0.00409806 | 0.00499809 |
| 40 | 0.99918378 | 0.99918378 | 0.00062544 | 0.00062538 |
| 45 | 0.99987590 | 0.99987590 | 0.00009436 | 0.00099432 |
| 50 | 0.99998123 | 0.99998123 | 0.00001416 | 0.00001414 |
| 55 | 0.99999717 | 0.99999717 | 0.00000212 | 0.00000211 |
| 60 | 0.99999958 | 0.99999958 | 0.00000032 | 0.00000031 |

${ }^{a}$ The errors in Figs. 4-6 are relative to these PWBA2 results for partial-wave numbers of 40, 50 , and 60.


Fig. 4. Dependence of errors in scattering matrix elements on integration step size for a 15 F matching radius.


Fig. 5. Dependence of errors in scattering matrix elements on integration step size for a 25 F matching radius.
$R_{M}=25$ F, Fig. 5 reveals scattering matrix errors growing as the fourth power of integration step size. This implies that the dominant source of error at large matching radii is accumulating truncation in the numerical integration. If, instead, the main source were round-off, the characteristic $H^{-2}$ dependence would be observed. Compilation of the modified GIBELUMP in double precision on a computer (the MSU Cyclotron Laboratory XDS Sigma-7) with 32-bit words is largely responsible for the lack of noticeable round-off error.

Similar studies have been made for $\ell=0$ and 10 by using $S_{\ell}$ 's from the modified GIBELUMP (with $R_{M}=25.0 \mathrm{~F}$ and $H=0.0125 \mathrm{~F}$ ) instead of PWBA2. The redefined "errors" in the scattering matrix show the same behavior as functions of $R_{M}$ and $H$ for low partial-wave number, as $\epsilon_{40}, \epsilon_{50}$, and $\epsilon_{60}$ in Figs. 3-5.

## IV. Errors in the Differential Cross Section

Thus far we have determined that a matching radius of about 25 F and the smallest integration step size consistent with our 2000 step maximum (computer memory limited), i.e., $H \approx 0.0125 \mathrm{~F}$, minimize the errors in our partial-wave amplitudes. The total error in the full elastic scattering amplitude also contains contributions from the aforementioned loss of significance (due to cancellation
in the partial-wave sum), and neglect of terms (in Eq. (2)) for $\ell$ greater than some $L_{\text {max }}$. Table I indicates that, much beyond $\ell=60$, the scattering matrix elements will differ from unity by less than their probable errors. Thus, there are vanishing returns from selecting $L_{\text {max }}$ above 60 . Also, it is found that Coulomb functions calculated with the modified GIBELUMP for $\ell=60, \eta=1.81733$, and $\rho=75$ ( $r \approx 25$ ) remain constant to 12 significant figures, when values greater than the previously used $\mathscr{L}=100$ and $L=101$ are tried. Note that this does not imply an accuracy of anything like one part in a trillion for the $F_{\ell}$ 's and $G_{\ell}$ 's, since the radius at which the semiconvergent asymptotic series are summed ( $\mathscr{R}$ ) is also important. A comparison of Coulomb functions from the modified GIBELUMP (for $\eta=0$ ) with Ricatti-Bessel functions from RBESS2 [20] suggests an accuracy more on the order of one part in a million. However, this will clearly not be improved by selecting values of $\mathscr{L}$ and $L$ larger than 100 and 101, respectively. Thus, we will refer to the following set as our "optimum numerical accuracy parameters'": $R_{M}=\mathscr{R}=25.0 \mathrm{~F}, H=0.0125 \mathrm{~F}, L_{\text {max }}=60, \mathscr{L}=100$, and $L=101$. Assuming they yield a sufficiently accurate scattering amplitude at 71 MeV , for the full (including Coulomb) ${ }^{3} \mathrm{He}^{-60} \mathrm{Ni}$ potential, allows us to define an "error" in the differential cross section by

$$
\epsilon(\theta)=\frac{\left|\sigma_{0}(\theta)-\sigma_{T}(\theta)\right|}{\sigma_{0}(\theta)} \times 100 \%,
$$

where $\sigma_{0}(\theta)$ is calculated by the modified GIBELUMP with the optimum parameters and $\sigma_{T}(\theta)$, with some test set. A few values of $\sigma_{0}(\theta)$ are listed in Table II.

Investigating this error as a function of $R_{M}, H$, and $L_{\text {max }}$, for several scattering angles $(\theta)$ of interest, affords a means of minimizing calculation time, by selecting parameters which yield sufficient accuracy, but not greater than required. For example, it might be a very inefficient use of computer time to calculate cross sections accurate to 6 significant figures, while searching on data with $10 \%$ experimental errors. In studying $\epsilon(\theta)$, the test parameters were varied one at a time, the others remaining fixed at their optimum values. ${ }^{1}$
All optical-model codes have limits on the values of the numerical accuracy parameters. Most also have internal criteria which choose some of them automatically. The codes of Fig. 2 selected matching radii between 10 F and 13 F for $71 \mathrm{MeV}^{3} \mathrm{He}$ scattering from the potential defined by Eq. (1). The original GIBELUMP sets $R_{M}$ equal to the radius plus seven times the diffuseness of whichever term in the potential gives the largest value. GENOA does the same, but uses nine times the diffuseness. If it is not externally specified, SNOOPY3 defines the matching radius to be the point at which the ratio of nuclear to Coulomb potential is $0.005 / \mathrm{k}$. DWUCK adds the largest radius (of any term in

[^1]TABLE II
$71 \mathrm{MeV}{ }^{3} \mathrm{He}$ Elastic Scattering from ${ }^{60} \mathrm{Ni}$ as Calculated with the Modified GIBELUMP for the Optical-Model and Optimum Numerical Accuracy

Parameters Defined in the Text ${ }^{a}$

| $\theta_{\text {o.m. } .}(\mathrm{deg})$ | $\sigma_{\sigma . \mathrm{m} .}(\mathrm{mb} / \mathrm{sr})$ |
| :---: | :---: |
| 10.0 | $4.942 \times 10^{3}$ |
| 20.0 | $9.444 \times 10^{1}$ |
| 30.0 | $1.334 \times 10^{1}$ |
| 40.0 | $7.929 \times 10^{-1}$ |
| 50.0 | $1.342 \times 10^{-1}$ |
| 60.0 | $1.849 \times 10^{-1}$ |
| 70.0 | $7.996 \times 10^{-2}$ |
| 80.0 | $2.551 \times 10^{-2}$ |
| 90.0 | $8.972 \times 10^{-3}$ |
| 100.0 | $2.970 \times 10^{-8}$ |
| 110.0 | $7.659 \times 10^{-4}$ |
| 120.0 | $2.217 \times 10^{-4}$ |
| 130.0 | $8.363 \times 10^{-5}$ |
| 140.0 | $2.818 \times 10^{-5}$ |
| 150.0 | $1.112 \times 10^{-5}$ |
| 160.0 | $4.462 \times 10^{-6}$ |
| 170.0 | $2.241 \times 10^{-6}$ |
| 180.0 | $2.596 \times 10^{-5}$ |

${ }^{a}$ The errors in Figs. 6-8 have been determined with respect to these cross sections at 90.0 , $150.0,170.0$, and 180.0 degrees.
the potential) to 9.2 times the largest diffuseness. Figure 6 illustrates that these criteria yield matching radii which are too small for the modified GIBELUMP to accurately calculate our back-angle cross sections. Also note that the errors are growing exponentially beyond 27 F .

Hodgson has suggested that each unit of $\rho$ be divided into 10 integration steps [21]. This gives a step size of about 0.03 F for the 71 MeV helions. Figure 7 indicates that this choice corresponds to only $0.1 \%$ errors in $\sigma(\theta)$, even at the largest angles. However, of the four codes we have examined, only SNOOPY3 has the capability of selecting $H$ (with a more complicated method than Hodgson's). For the calculation shown in Fig. 2, SNOOPY3 picked $H=0.05$ F, the smallest value which it allows. The other three codes were given the commonly used 0.1 F integration step size, which, alone, would be responsible for up to $10 \%$ errors in the cross section (Fig. 7).


Fig. 6. Dependence of errors in $\sigma(\theta)$ on matching radius, with other accuracy parameters at optimum values, e.g., $H=0.0125 \mathrm{~F}$ and $L_{\max }=60$.


Fig. 7. Dependence of errors in $\sigma(\theta)$ on integration step size, with other accuracy parameters at optimum values, e.g., $R_{M}=25.0 \mathrm{~F}$ and $L_{\text {max }}=60$.

Criteria similar to Hodgson's for the number of partial waves [21] have been widely incorporated into optical-model codes. GENOA, the original GIBELUMP, and SNOOPY3 all truncate the partial-wave sum after some condition closely related to $\left|1-S_{\ell}\right|<10^{-N}$ is satisfied. For GENOA and the original GIBELUMP, $N=4$, and for SNOOPY3, $N=3$, if not otherwise specified. Each of these codes used $33 \leqslant L_{\max } \leqslant 37$ for the calculations of Fig. 2. The DWBA code, DWUCK, requires the user to input the number of partial waves to be included in the sum. For this comparison with the optical-model codes, we let $L_{\max }=35$ for DWUCK. However, from Fig. 8 we conclude that enormous errors in the small, back-angle cross sections can result from the neglect of partial waves above the thirty-fifth.


Fig. 8. Dependence of errors in $\sigma(\theta)$ on the number of partial waves included in the sum, with other accuracy parameters at optimum values, e.g., $R_{M}=25.0 \mathrm{~F}$ and $H=0.0125 \mathrm{~F}$.

## V. Conclusion

The disagreement between codes depicted in Fig. 2 may be greatly diminished by the use of improved values for the numerical accuracy parameters. In particular, increasing (within limits) the matching radii and numbers of partial waves from the values employed in the original GIBELUMP, GENOA, SNOOPY3, and DWUCK calculations of Fig. 2 would yield cross sections approaching the angular
distribution obtained from the modified GIBELUMP with the optimum numerical accuracy parameters. To a lesser extent, decreasing the integration step sizes would also help. Figure 9 illustrates, as an example, the effect of using DWUCK with $R_{M}=20.0 \mathrm{~F}, L_{\max }=60$, and $H=0.05 \mathrm{~F}$, rather than $R_{M}=12.65 \mathrm{~F}$, $L_{\max }=35$, and $H=0.10 \mathrm{~F}$, as in Fig. 2. In both of these figures, the solid lines are $\sigma_{0}(\theta)$, as calculated with the modified GIBELUMP and the optimum numerical accuracy parameters (e.g., $R_{M}=25.0 \mathrm{~F}, L_{\max }=80$, and $H=0.0125 \mathrm{~F}$ ). The vastly closer agreement of the GIBELUMP and DWUCK calculations in Fig. 9


FIG. 9. Elastic scattering calculated with the modified GIBELUMP, for the optimum numerical accuracy parameters defined in the text, and with DWUCK, for parameters as near these as possible. Compare with Fig. 2.
than in Fig. 2 provides further evidence that parameters approaching our optimum values yield considerably greater numerical accuracy than those commonly used in optical-model codes for ${ }^{3} \mathrm{He}$ elastic scattering, especially for the small, backangle cross sections which occur for bombarding energies on the order of 70 MeV . Note that the pronounced, back-angle oscillations in the original GIBELUMP, GENOA, SNOOPY3, and DWUCK angular distributions of Fig. 2 are replaced (except for the "glory peak" [22]) by a smooth fall in the more accurate calculations. This behavior bears a strong qualitative resemblance to the data in Fig. 1, and may be expected to facilitate the optical-model analyses.

This investigation has concentrated on a particular example of elastic scattering. No attempt has been made to suggest new criteria for the numerical accuracy parameters which would be adequate over wide ranges of projectiles, targets,
and energies. Each case deserves individual attention. However, we trust that these results are indicative of the numerical difficulties associated with using standard optical-model codes to calculate small cross sections.

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[^1]:    ${ }^{1}$ For matching radii greater than $25 \mathrm{~F}, H=0.015 \mathrm{~F}$ was used, rather than $H=0.0125 \mathrm{~F}$.

