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Gaussian expansions in distorted-wave–Born-approximation calculations

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The use of Gaussian expansions for the bound-state functions in distorted-wave–Born-approximation calculations is discussed. The use of these expansions leads to an analytic expression for the form factor which can be used to simplify the numerical evaluation of the matrix element. In addition, the Gaussian functions are useful when studying the structure of the form factor. In particular, the validity of the "no-recoil" approximation is discussed and a semiclassical interpretation is presented. A computer program (GAUSS) using the Gaussian expansions has been developed and used to evaluate the cross sections of some previously studied reactions. Comparisons of the results with those of other programs are given.

[NUCLEAR REACTIONS Full-recoil DWBA, Gaussian expansions.]

I. INTRODUCTION

The distorted-wave–Born-approximation (DWBA) is an important tool for analyzing nuclear transfer reactions, but the numerical evaluation of the six-dimensional integral in the transition amplitude is difficult and tedious. If the DWBA analysis is to be a useful tool one must either use an efficient method for evaluating the integral or use valid approximations which simplify the numerical integration. A good understanding of the form factor in the integral is required before an approximation can be used with confidence. Presently there are several techniques for the numerical evaluation of the integral,[1-5] and there exist several forms of the "no-recoil" and "zero-range" approximations for simplifying the integral.[6-9] When these various approximations are valid is a question which is still being investigated.[10,11]

In this paper a new technique is presented for the numerical evaluation of the "exact finite-range" DWBA matrix element. The technique consists of expanding the bound-state wave functions as a series of Gaussian functions. This expansion not only simplifies the calculation of the form factor, but it can also be used to gain a better understanding of the structure of the form factor. Hopefully, a better understanding of the form factor can be used to determine when various approximations are valid. In addition, once the bound states have been expressed as a sum of Gaussian functions, it is easy to transform the form factor to another desired set of coordinates.

While several DWBA programs[3-5,8,12-14] already exist using the methods in Ref. 1, it is useful to have an alternative method. The method presented in this paper not only provides a useful check for the existing programs, but it also may be more efficient for some reactions. The question of which method should be used will be decided by experience in using the various programs. There have been many papers[8,10,12-14] discussing the properties of the existing programs; some comparisons of the present program with these published results are presented.

One advantage of the present method is that the form factor is an analytic function of the Gaussian expansion parameters. Thus, once an accurate expansion of the bound states has been obtained, no numerical integrations are required to generate the partial-wave expansion of the form factor. Also, since the form factor is expressed in terms of the expansion parameters, only a small amount of computer core storage is required. Another advantage is that the present method can be generalized in a straightforward way to handle the transfer of more than one cluster.

Gaussian expansions can also be used to investigate the failings of the no-recoil and zero-range approximations. While it is well known that the use of no-recoil approximations can result in unphysical oscillations in the differential cross section, there is another aspect of this approximation which has not been discussed previously. This is the failure of the no-recoil approximation to produce a forward-peaked angular distribution for transfer reactions with nonzero values of the angular momentum transfer. This aspect of the no-recoil approximation was discovered during attempts to fit ^{12}C(^{7}Li, t)^{16}O angular distributions. Data for this reaction are forward peaked, but no-recoil DWBA predictions were not forward peaked for any reasonable set of optical-model parameters at the energies which were investigated. However, using a finite-range DWBA program which included recoil effects, the calculated distribution was found to be forward peaked. This effect is especially puzzling since the differential cross section was found to be strongly forward peaked in previous no-recoil calculations for the ^{12}C(^{6}Li, d)^{16}O reaction, in agreement with experi-

mental results. For both types of reactions an α particle is transferred to the same state in ^{16}O; the only essential difference between the $(^7Li, t)$ and the $(^6Li, d)$ reactions is that for ^7Li the α particle and the triton are bound in a p state, while for ^6Li the α particle and the deuteron are bound in an s state. Thus, if the α particle is transferred to an s state in ^{16}O, the angular momentum transfer is unity for the $(^7Li, t)$ reaction and zero for the $(^6Li, d)$ reaction. In this paper the Gaussian expansions are used to present a qualitative semiclassical explanation for these forward-angle effects as well as a quantum-mechanical discussion of the results.

In Sec. II the Gaussian expansions are used to give a simple expression for the form factor. In Sec. III the form factor for a particular set of reactions is studied, and in Sec. IV the results of the present program are compared with those of several established programs.

II. DWBA THEORY

Following Austern *et al.*[1] we consider $A(a,b)B$ reaction, where the incident beam particles a consist of a core b, with angular momentum s_b, bound to the cluster x, with angular momentum j_x; and in the final channel the particle B consists of the core A with angular momentum J_A, bound to the cluster x. The total angular momentum of a is s_a and the total angular momentum of B is J_B. The coordinates used to describe the reaction are shown in Fig. 1.

For simplicity we consider the case where the bound states of x have only one value of total and orbital angular momentum; we assume for the initial state

$$\vec{j}_1 = \vec{l}_1 + \vec{j}_x$$

and for the final state

$$\vec{j}_2 = \vec{l}_2 + \vec{j}_x \ .$$

For a spin-independent interaction the selection rules for total, spin, and orbital transferred angular momenta are:

$$\begin{aligned} \vec{j} &= \vec{J}_B - \vec{J}_A = \vec{j}_2 \ , \\ \vec{s} &= \vec{s}_a - \vec{s}_b = \vec{j}_1 \ , \\ \vec{l} &= \vec{j}_2 - \vec{j}_1 = \vec{l}_2 - \vec{l}_1 \ . \end{aligned} \tag{1}$$

A. Recoil

The cross section with recoil included is given as an incoherent sum over s, j, l, and m of the partial amplitudes $\beta_{sj}^{lm}(\vec{k}_b, \vec{k}_a)$, where[1]

$$(2l+1)^{1/2} i^l \beta_{sj}^{lm}(\vec{k}_b, \vec{k}_a) = \int d\vec{r}_a \int d\vec{r}_b \chi_b^{(-)*}(\vec{k}_b, \vec{r}_b) f_{lsjm}(\vec{r}_b, \vec{r}_a) \chi_a^{(+)}(\vec{k}_a, \vec{r}_a) \tag{2}$$

and $\chi^{(+)}$ ($\chi^{(-)}$) is the incoming (outgoing) distorted wave. Dropping the s and j subscripts, the post interaction form factor is given by

$$f_{lm}(\vec{r}_b, \vec{r}_a) = (-1)^{l_1 + j_x + j_2 + m} (2l+1) i^l \left(\frac{2s_a+1}{2l_1+1}\right)^{1/2} \times \sum_{m_1, m_2} (l_2 m_2 lm | l_1 m_1) W(l_1 j_1 l_2 j_2; j_x l) [\varphi_{l_2}^{m_2}(\vec{r}_{Ax})]^* [V(r_{bx}) + V(r) - U_b(r_b)] \varphi_{l_1}^{m_1}(\vec{r}_{bx}) \ . \tag{3}$$

Here $\varphi_{l_1}^{m_1}(\vec{r}_{bx})$ is the initial bound-state wave function, $\varphi_{l_2}^{m_2}(\vec{r}_{Ax})$ is the final bound-state wave function, and $U_b(r_b)$ is the distorting potential for the final channel. For simplicity we consider only the $V(r_{bx})$ potential. Using

$$\vec{r}_{Ax} = \left(1 - \frac{Ab}{Ba}\right)^{-1} \left(\vec{r}_a - \frac{b}{a}\vec{r}_b\right) \tag{4}$$

and

$$\vec{r}_{bx} = \left(1 - \frac{Ab}{Ba}\right)^{-1} \left(\frac{A}{B}\vec{r}_a - \vec{r}_b\right) \tag{5}$$

Eq. (3) can be written as an explicit function of $\vec{r}_a$ and $\vec{r}_b$. The symbols a, b, A, and B stand for the mass of the corresponding particle.

Austern *et al.*[1] showed that the six-dimensional integral in Eq. (2) can be reduced to a sum of lower-dimensional integrals by using the partial-wave expansion of the distorted waves and writing the form factor as

$$f_{lm}(\vec{r}_b, \vec{r}_a) = \sum_{L_a L_b M} F_{lL_a L_b}(r_b, r_a) Y_{L_b}^{M*}(\hat{r}_b) \times Y_{L_a}^{m-M*}(\hat{r}_a) (L_b M L_a m - M | lm). \tag{6}$$

The evaluation of the transition matrix element is thereby reduced to the sum of the two-dimensional integrations over r_a and r_b; in practice, $F_{lL_a L_b}$ is usually determined by the numerical evaluation

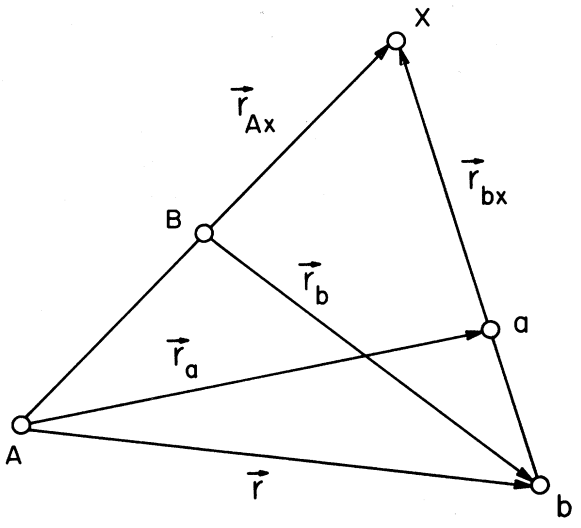

FIG. 1. The coordinate vectors for the $A(a, b)B$ reaction.

of an integral for each value of r_a and r_b. In this case the evaluation of the matrix element is in reality a sum of three-dimensional integrals.

As pointed out by Austern *et al.*,[1] if the bound-state wave functions have a Gaussian form, then the quantities $F_{lL_aL_b}$ can be determined analytically. Since the Gaussians form a complete set,[15,16] we expand the bound-state functions as sums of Gaussians, i.e., we write

$$V(r_{bx})\varphi_{l_1}^{m_1}(\vec{r}_{bx}) = \sum_{i=1}^{I} c_i(\gamma_i r_{bx})^{l_1} \times \exp(-\gamma_i^2 r_{bx}^2) Y_{l_1}^{m_1}(\hat{r}_{bx}) \quad (7a)$$

and

$$\varphi_{l_2}^{m_2}(\vec{r}_{Ax}) = \sum_{n=1}^{N} d_n(\lambda_n r_{Ax})^{l_2} \times \exp(-\lambda_n^2 r_{Ax}^2) Y_{l_2}^{m_2}(\hat{r}_{Ax}) . \quad (7b)$$

Such expansions have been used previously in atomic- and nuclear-physics calculations.[15,17,18] It has been shown[16] that, when using expansions of this type, only a few terms are needed for accurate approximations for the bound-state functions. In Sec. III the exact and approximation functions for the $^{12}C(^7Li, t)^{16}O$ and $^{12}C(^6Li, d)^{16}O$ reactions are compared.

Austern *et al.*[1] write the bound-state functions in the form

$$\varphi_{l_1}^{m_1}(\vec{r}_{bx}) = i^{l_1}\omega_{l_1}(r_{bx})[r_{bx}{}^{l_1} Y_{l_1}^{m_1}(\hat{r}_{bx})] \quad (8a)$$

and

$$\varphi_{l_2}^{m_2}(\vec{r}_{Ax}) = i^{l_2}\omega_{l_2}(r_{Ax})[r_{Ax}{}^{l_2} Y_{l_2}^{m_2}(\hat{r}_{Ax})] , \quad (8b)$$

where the "kernel" of the form factor is given by

$$g_K(r_a, r_b) = \int_{-1}^{1} d\mu\, \omega_{l_2}(r_{Ax}) V(r_{bx}) \omega_{l_1}(r_{bx}) P_K(\mu).$$

From Eqs. (7) and (8) one finds

$$g_K(r_a, r_b) = \sum_i \sum_n (c_i \gamma_i{}^{l_1})(d_n \lambda_n{}^{l_2}) \times \int_{-1}^{+1} d\mu \exp(-\lambda_n^2 r_{Ax}{}^2 - \gamma_i^2 r_{bx}{}^2) P_K(\mu) ,$$

where μ is the cosine of the angle between $\vec{r}_a$ and $\vec{r}_b$. Using Eqs. (4) and (5) to write

$$\gamma_i \vec{r}_{bx} = \alpha_i \vec{r}_a - \beta_i \vec{r}_b , \quad (9a)$$

$$\lambda_n \vec{r}_{Ax} = \epsilon_n \vec{r}_a - \nu_n \vec{r}_b \quad (9b)$$

the exponential term in the integral can be rewritten in the form

$$\exp[-(\alpha_i^2 + \epsilon_n^2) r_a^2 - (\beta_i^2 + \nu_n^2) r_b^2 + 2(\alpha_i\beta_i + \epsilon_n\nu_n)\vec{r}_a \cdot \vec{r}_b] .$$

From the addition theorem for the last term in the exponential one finally obtains

$$g_K(r_a, r_b) = \sum_i \sum_n (c_i \gamma_i{}^{l_1})(d_n \lambda_n{}^{l_2}) \exp[-(\alpha_i^2 + \epsilon_n^2) r_a^2 - (\beta_i^2 + \nu_n^2) r_b^2] \left(\frac{\pi}{(\alpha_i\beta_i + \epsilon_n\nu_n) r_a r_b}\right)^{1/2} \times I_{K+1/2}(2(\alpha_i\beta_i + \epsilon_n\nu_n) r_a r_b) , \quad (10)$$

where $I_{K+1/2}$ is the modified spherical Bessel function of the first kind.

Using Eq. (10) above in Eq. (57) of Austern *et al.*,[1] one obtains an analytic expression for the form factor for all r_a and r_b. Since the form factor can be expressed analytically for Gaussian functions, the use of the Gaussian expansions reduces the problem of the evaluation of the transition matrix element to one of determining a limited number of two-dimensional integrals. This is where the present approach differs significantly from the full-recoil approach of Sawaguri and Tobocman,[6] who expand the bound states in harmonic oscillator (HO) functions. Using the HO addition theorem, the form factor is then expressed in terms of an infinite sum of products of

functions of r_a and functions of r_b. This sum must be truncated when the desired convergence is obtained. While their method reduces the form factor to a sum of products of one-dimensional integrals, the convergence can be quite slow.

B. No-recoil and zero-range approximations

The use of Gaussian expansions aids in the study of the applicability and physical significance of various commonly made approximations such as the no-recoil and zero-range approximations. There are several variations of the no-recoil approximation, but in the limit where the mass of x is much smaller than the masses of A and b they are equivalent. The two most common forms are those of Sawaguri and Tobocman[6] and of Dodd and Greider.[7] Dodd and Greider use

$$\vec{r}_a = \vec{r} + \frac{x}{a}\vec{r}_{bx} \approx \vec{r}$$

and

$$\vec{r}_b = \frac{A}{B}\vec{r} - \frac{x}{B}\vec{r}_{bx} \approx \frac{A}{B}\vec{r}$$

to simplify the numerical evaluation of the integral in Eq. (2), while Sawaguri and Tobocman use

$$\vec{r}_b = \frac{A}{B}\vec{r}_a - \frac{x(A+b+x)}{Ba}\vec{r}_{bx} \approx \frac{A}{B}\vec{r}_a .$$

Both of these approximations reduce the evaluation of the integral to the sum of one-dimensional integrals. In this paper we consider only the Sawaguri and Tobocman approximation.

The approximation, as usually made, consists in replacing $\vec{r}_b$ with $(A/B)\vec{r}_a$ in the argument of the outgoing distorted wave, but retaining $\vec{r}_{bx}$ in the form factor. Integration of the form factor over $\vec{r}_b$, or equivalently $\vec{r}_{bx}$, for each value of $\vec{r}_a$, produces a function of $\vec{r}_a$ which is used to obtain a finite-range evaluation of the transition matrix element.

The validity of the no-recoil approximation is dependent upon the continuum wave functions. The Sawaguri and Tobocman approximation will be valid if

$$\chi_b^{(-)}(\vec{k}_b, \vec{r}_b) \approx \chi_b^{(-)}\left(\vec{k}_b, \frac{A}{B}\vec{r}_a\right)$$

over the range of values where the form factor is non-negligible. The size of this region depends upon the bound-state wave functions. If R_I is the radius of this region and K is the local wave number of the outgoing distorted wave, the approximation is valid for

$$\left(\frac{A}{a}+1\right)\left(\frac{A}{x}+1\right)^{-1}(KR_I) \ll 1 . \qquad (11)$$

This is true if the range of the interaction is small, as in the (d,p) reactions, or if the energy is low, so that the local wave number is small. Neither of these characteristics is present, for instance, in the $^{12}C(^7Li, t)^{16}O$ and $^{12}C(^6Li, d)^{16}O$ reactions.

If the interaction $V(r_{bx})$ is very-short range, it may be possible to replace it with a δ function, giving a zero-range evaluation of the transition matrix element. Zero range, of course, includes the no-recoil approximation. In order to illustrate the properties of the Gaussian expansions in more detail the form factor is now considered for two particular reactions.

III. $^{12}C(^7Li, t)^{16}O$ AND $^{12}C(^6Li, d)^{16}O$ FORM FACTORS

We consider the case where the α particle is bound in an s state in ^{16}O. For this case there is only one value of the transferred angular momentum l and this is the angular momentum of the α particle in the initial channel; thus $l=1$ for ^7Li and $l=0$ for ^6Li. Since there is only one value of the transferred angular momentum, the differences between the no-recoil and the complete DWBA cannot be caused by neglected values of l. We show that the differences are caused by the no-recoil restriction that $\vec{r}_b$ is a constant times $\vec{r}_a$.

For $l_2=0$ and $j_2=0$ the form factor becomes

$$f_{l_1 m_1}(\vec{r}_b, \vec{r}_a) = (-1)^{l_1+m_1} i^{l_1} (2s_a+1)^{1/2} \times \varphi_{l_2}^{m_2}(\vec{r}_{Ax}) V(r_{bx}) \varphi_{l_1}^{m_1}(\vec{r}_{bx}) . \qquad (12)$$

The Gaussian expansions for $\varphi_{l_2}^{m_2}$ and $V\varphi_{l_1}^{m_1}$ are obtained by a χ^2 fit of the sums in Eqs. (7a) and (7b) to the corresponding expressions for a Woods-Saxon well. In order to fit the function over its entire range, and not to overemphasize zero-crossing values, each point is weighted by the inverse of the average of the wave function at this point and at its nearest neighbors. Parameters for Gaussian expansions and their χ^2 values are listed in Tables I and II. Equally spaced sets of the exponent parameters γ_i and λ_n are shown in the tables. The use of equally spaced coefficients serves to speed up the computer program but is not essential to the use of Gaussian expansions. The bound-state potentials are the same as those used by Kubo and Hirata.[8] Comparisons of the bound-state functions with their Gaussian expansions are given in Figs. 2–5. These figures show that the sum of a small number of Gaussians provides a good approximation for the bound-state functions.

The real test of the validity of the expansion is whether or not the approximate form factor gives

TABLE I. Parameters for the Gaussian expansions of $V\varphi(^7\mathrm{Li})$ and $\varphi(^{16}\mathrm{O}, \text{g.s.})$.

	$V\varphi$ for $^7\mathrm{Li}(\alpha+t)$		φ for $^{16}\mathrm{O}(\alpha+^{12}\mathrm{C})$	
i	c_i	γ_i	d_n	λ_n
n	(MeV fm$^{-3/2}$)	(fm^{-1})	(fm$^{-3/2}$)	(fm^{-1})
1	1.104 571 6D − 04	0.240 931 10	6.866 915 5D − 04	0.191 712 05
2	1.393 835 4D − 01	0.352 624 10	4.006 582 3D − 02	0.258 672 75
3	5.764 996 7	0.464 317 10	9.547 821 9D − 01	0.325 633 45
4	1.827 578 1D + 01	0.576 010 10	2.161 818 2	0.392 594 15
5	9.509 121 1D + 01	0.687 703 09	−8.698 323 5	0.459 554 85
6	−2.015 279 2D + 02	0.799 396 09	3.506 339 9D + 01	0.526 515 55
7			−6.543 042 8D + 01	0.593 476 25
8			3.821 725 7D + 01	0.660 436 95
	$\chi^2 = 1.23D - 04$		$\chi^2 = 1.77D - 04$	

the correct differential cross section. Figure 6 shows a comparison of the plane-wave cross section obtained using the exact bound-state wave functions with the cross section obtained using the approximate Gaussian expansions. For this case, where the cross section can be computed from the Fourier transforms of the bound-state functions, the agreement is excellent. This comparison is a good check of the method (and program) because the two calculations are done in quite different manners.

To study the shape of the form factor, Eqs. (7), (9), and (12) and the addition theorem for spherical harmonics are used to write

$$f_{l_1 m_1}(\vec{r}_b, \vec{r}_a) = (-1)^{l_1+m_1} i^{l_1} (2s_a+1)^{1/2} \sum_{i,n} c_i d_n \exp[-(\alpha_i^2+\epsilon_n^2) r_a^2 - (\beta_i^2+\nu_n^2) r_b^2 + 2(\alpha_i\beta_i + \epsilon_n\nu_n)\vec{r}_a \cdot \vec{r}_b]$$
$$\times \sum_{\lambda\mu} \left[\frac{(2l_1+1)!}{(2\lambda+1)!(2l_1-2\lambda+1)!}\right]^{1/2} (\alpha_i r_a)^{l_1-\lambda} (\beta_i r_b)^{\lambda}$$
$$\times (l_1 - \lambda\, m_1 - \mu\, \lambda\mu \,|\, l_1 m_1) Y_{l_1-\lambda}^{m_1-\mu}(\hat{r}_a)(-1)^{\lambda} Y_{\lambda}^{\mu}(\hat{r}_b). \tag{13}$$

We first consider the (^{6}Li, d) case which has $l_1 = 0$. Equation (13) can be written as

$$f_{00}(\vec{r}_b, \vec{r}_a) = \sqrt{3} \sum_{i,n} \frac{c_i d_n}{4\pi} \exp\left[-(\alpha_i^2+\epsilon_n^2) r_a^2 + \frac{(\alpha_i\beta_i+\epsilon_n\nu_n)^2}{\beta_i^2+\nu_n^2} r_a^2\right] \exp\left[-(\beta_i^2+\nu_n^2)\left(\vec{r}_b - \frac{\alpha_i\beta_i+\epsilon_n\nu_n}{\beta_i^2+\nu_n^2}\vec{r}_a\right)^2\right] \tag{14}$$
$$= \sum_{i,n} D_{in}(r_a) \exp\left[-(\beta_i^2+\nu_n^2)\left(\vec{r}_b - \frac{\alpha_i\beta_i+\epsilon_n\nu_n}{\beta_i^2+\nu_n^2}\vec{r}_a\right)^2\right]. \tag{15}$$

TABLE II. Parameters for the Gaussian expansions of $V\varphi(^6\mathrm{Li})$ and $\varphi(^{16}\mathrm{O}, 6.06\ \mathrm{MeV})$.

	$V\varphi$ for $^6\mathrm{Li}(\alpha+d)$		φ for $^{16}\mathrm{O}^*(\alpha+^{12}\mathrm{C})$	
i	c_i	γ_i	d_n	λ_n
n	(MeV fm$^{-3/2}$)	(fm^{-1})	(fm$^{-3/2}$)	(fm^{-1})
1	2.429 110 0D − 01	0.307 570 86	1.091 256 2D − 03	0.117 223 23
2	1.281 290 9	0.400 896 46	6.773 239 1D − 02	0.185 721 75
3	7.797 410 5	0.494 222 05	4.295 619 7D − 03	0.254 220 26
4	1.245 814 0D + 01	0.587 547 65	1.998 254 0	0.322 718 77
5	8.686 561 4D + 01	0.680 873 25	2.030 307 4	0.391 217 28
6	−1.684 312 4D + 02	0.774 198 84	−6.270 376 2D + 01	0.459 715 79
7			3.490 746 7D + 02	0.528 214 31
8			−1.068 859 7D + 03	0.596 712 82
9			1.769 267 8D + 03	0.665 211 33
10			−1.464 596 5D + 03	0.733 709 84
11			4.752 478 8D + 02	0.802 208 36
	$\chi^2 = 1.75D - 04$		$\chi^2 = 2.55D - 03$	

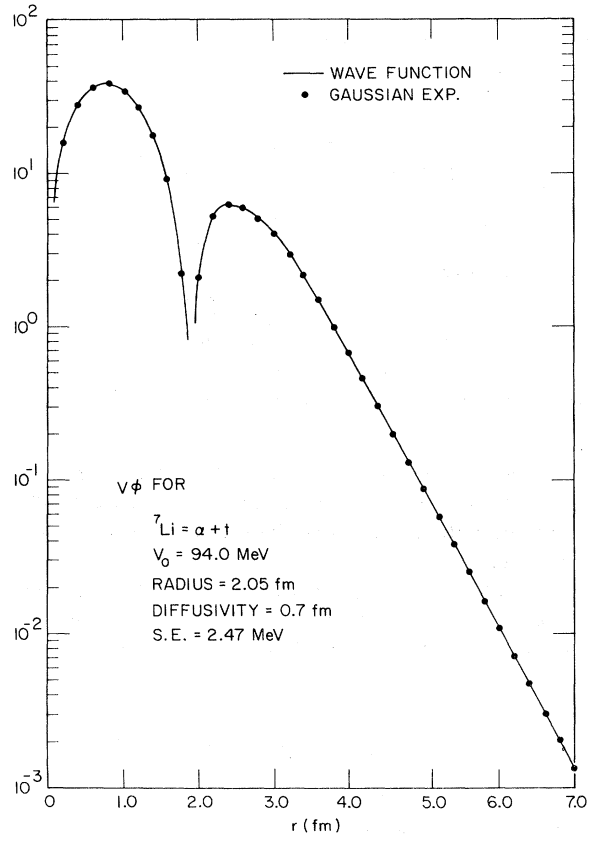

FIG. 2. Comparison of $V\varphi$ for ^{7}Li ($l_1 = 1$) with the Gaussian expansion. The bound-state wave function was obtained by numerical integration of the Schrödinger equation with both a Coulomb potential and a Woods-Saxon nuclear potential. Only the nuclear potential is included in V in the product $V\varphi$.

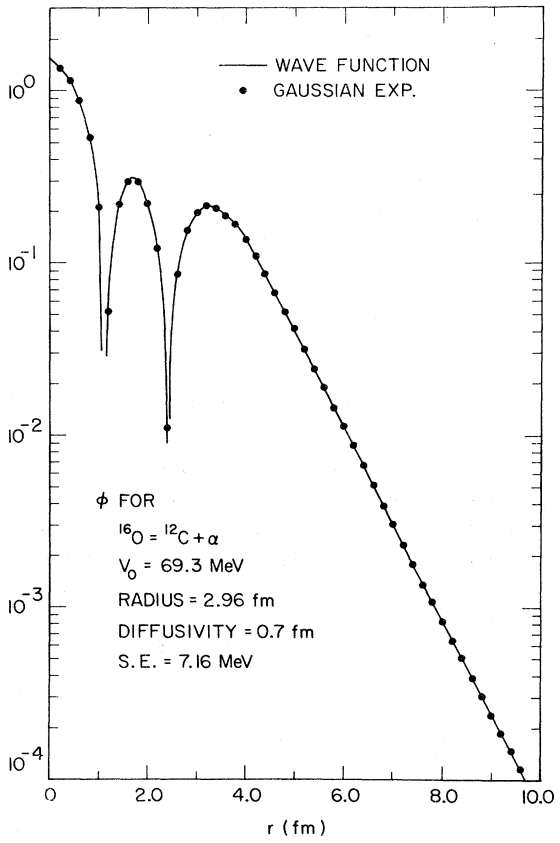

FIG. 3. Comparison of φ for ground-state ^{16}O ($l_2 = 0$) with the Gaussian expansion. The bound-state wave function was obtained by numerical integration of the Schrödinger equation with both a Coulomb potential and a Woods-Saxon nuclear potential.

Each term in the form factor depends on the directions of $\vec{r}_a$ and $\vec{r}_b$ in the form of an exponential

$$\exp[-\xi_{in}(\vec{r}_b - \eta_{in}\vec{r}_a)^2] .$$

For a fixed value of $\vec{r}_a$ each term in this sum is peaked at

$$\vec{r}_b = \eta_{in}\vec{r}_a = \frac{\alpha_i\beta_i + \epsilon_n\nu_n}{\beta_i^2 + \nu_n^2}\vec{r}_a ; \tag{16}$$

this corresponds to $\vec{r}_b$ and $\vec{r}_a$ being collinear and lying on the line joining A and b. The sharpness of this peak is determined by

$$\beta_i^2 + \nu_n^2 = \left[\frac{B}{x(B+b)}\right]^2 [(\gamma_i a)^2 + (\lambda_n b)^2] . \tag{17}$$

In the limit of small transferred mass, one can see from (17) that this peak approaches a δ function and that

$$\eta_{in} = \frac{\alpha_i\beta_i + \epsilon_n\nu_n}{\beta_i^2 + \nu_n^2} = \frac{A}{B}\left[\frac{\gamma_i^2 + (Bb/Aa)\lambda_n^2}{\gamma_i^2 + (b/a)^2\lambda_n^2}\right] \to \frac{A}{B}, \tag{18}$$

which is the usual zero-range result. Also, if γ_i is large, one obtains the zero-range result. From (15) one can see that even if the transferred mass is not small the form factor has its largest values when $\vec{r}_b$ is parallel to $\vec{r}_a$, which is the justification of the finite-range no-recoil result. This is not the case for $l_1 \neq 0$.

We now consider the case for (^{7}Li, t) with $l_1 = 1$, $m_1 = 0$; for this case Eq. (13) can be written as

$$f_{10}(\vec{r}_b, \vec{r}_a) = -\sum_{i,n}\frac{\sqrt{-3}}{2\pi}c_i d_n \exp\left[-(\alpha_i^2 + \epsilon_n^2)r_a^2 + \frac{(\alpha_i\beta_i + \epsilon_n\nu_n)}{\beta_i^2 + \nu_n^2}r_a^2\right]\exp\left[-(\beta_i^2 + \nu_n^2)\left(\vec{r}_b - \frac{\alpha_i\beta_i + \epsilon_n\nu_n}{\beta_i^2 + \nu_n^2}\vec{r}_a\right)^2\right]$$
$$\times(\alpha_i r_a - \beta_i r_b\cos\theta) \tag{19}$$

$$= (r_b\cos\theta - \frac{A}{B}r_a)\sum_{i,n}\sqrt{-4}\,\beta_i D_{in}(r_a)\exp\left[-(\beta_i^2 + \nu_n^2)\left(\vec{r}_b - \frac{\alpha_i\beta_i + \epsilon_n\nu_n}{\beta_i^2 + \nu_n^2}\vec{r}_a\right)^2\right], \tag{20}$$

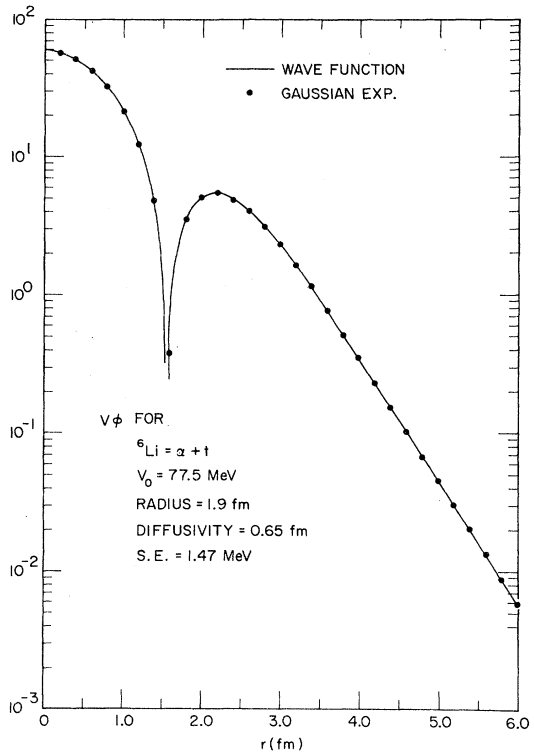

FIG. 4. Comparison of $V\varphi$ for ^{6}Li ($l_1 = 0$) with the Gaussian expansion. Cf. Fig. 2 caption.

where θ is the angle between $\vec{r}_a$ and $\vec{r}_b$. Each term in the form factor again depends on the directions of $\vec{r}_a$ and $\vec{r}_b$ in the form of an exponential, but now there is an additional factor in front of the sum which goes to zero in just those regions where the exponentials peak. The result is that, for fixed magnitudes of $\vec{r}_a$ and $\vec{r}_b$, Eq. (20) does not have its maximum value when $\vec{r}_a$ is parallel to $\vec{r}_b$. Consequently, the no-recoil approximation may be worse in this case. This also explains why modified zero-range interactions of the form

$$V\varphi = \delta(\vec{r}_b - t\vec{r}_a)$$

have not been successful for p-to-s-state transfer reactions.[19] The magnitude of the form factor f_{10} is actually at its minimum value for $\vec{r}_b = (A/B)\vec{r}_a$. This is also true for f_{11} since it is proportional to $\sin\theta$.

Classically, the explanation for the form factors is that when transferring a particle from one s state to another s state the particle must be moving along a line through the cores in both states resulting in transfer along a line through both cores. However, for transfer from a p state to an s state the transfer takes place along a line tangent to the initial orbit and directed toward the other core. This will not occur for the transferred particle on a line through the centers of the cores. The two cases are schematically illustrated in Fig. 7. Figure 7(a) shows A and a approaching each other in the center-of-mass system with a, made up of b and x, in an s state. Transfer is shown at the instant of closest approach but, in any case, when B consists of A and x in an s state, transfer will take place along the line joining A and a. Figure 7(b) shows the same situation except that a now consists of b and x in a p state resulting in transfer along the line shown. These classical trajectories correspond to maxima in the quantum-mechanical form factors discussed above.

Forward-angle cross sections are mainly determined by distant collisions or where r_a is large compared to the classical orbit of x in a. The classical pictures drawn in Fig. 7 correspond to the forward-angle cases. In the p-state to s-state case, the failure of no-recoil approximation to give proper forward-angle cross-section shape, let alone magnitude, is not surprising from the point of view of the classical analogy since it shows transfer occurs for $\vec{r}_b$ not parallel to $\vec{r}_a$. In fact, for large r_a no transfer occurs for $\vec{r}_b$ parallel to $\vec{r}_a$. Contour maps of the quantum-mechanical form factor confirm these classical pictures.

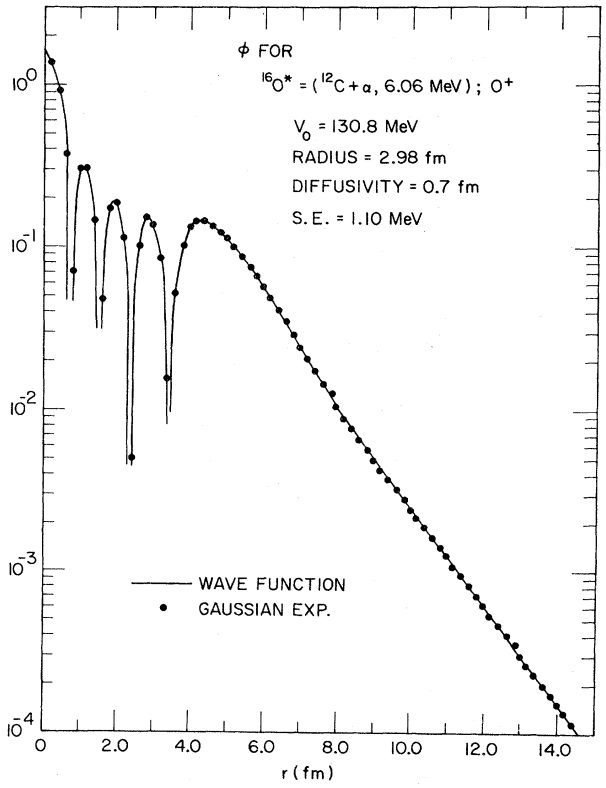

FIG. 5. Comparison of φ for excited-state ^{16}O ($l_2 = 0$) with the Gaussian expansion. Cf. Fig. 3 caption.

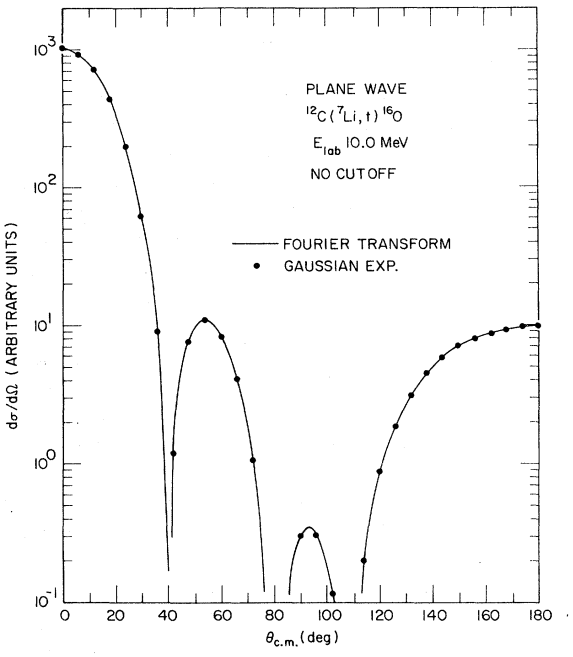

FIG. 6. Comparison of the plane-wave cross section obtained using the Fourier transforms of the bound-state wave functions with the plane-wave cross section obtained using the Gaussian expansions.

IV. GAUSS

A computer program (GAUSS) was written making use of the above described idea of Gaussian expansions to evaluate the differential cross section in the distorted-wave Born approximation. This program grew out of a no-recoil program which has been described elsewhere.[20] GAUSS was written to take advantage of the analytic form obtained for many of the expressions used in the evaluation, thereby reducing computer memory requirements.

GAUSS is divided into two parts. The first provides Gaussian expansions of $\varphi(\vec{r}_{Ax})$ and $V(\vec{r}_{bx})\varphi(\vec{r}_{bx})$. The number of Gaussians needed for accurate results depends on the complexity of the functions represented. Wave functions with up to six nodes have been fitted with no difficulty. The first part of the program also calculates the well depth of the Woods-Saxon well which will bind the given pair of particles together with the specified number of nodes in their wave function. This is done both for the incident and exit channels. Well radii and diffusivity are input parameters. The output of part one has already been shown in Figs. 2–5.

The second part uses the expansion parameters to evaluate the cross section and its running time depends linearly on the product of the number of Gaussians used in the two expansions. For the $^{12}C(^7Li, t)^{16}O$ reaction the running time for part one was 105 sec; for part two, 420 sec on an IBM 360/65. The effects of the ignored potentials in Eq. (3), $V(r)$ and $U_b(r_b)$, were investigated for this reaction by modifying GAUSS to include these potentials. This was relatively easy because of the technique of Gaussian expansion. Running time was essentially tripled and no significant changes were observed for the optical parameters used, so this subject was not pursued at this time. This result is consistent with the conclusions of DeVries, Satchler, and Cramer.[21]

Figure 8 shows the calculated differential cross sections for the $^{12}C(^7Li, t)^{16}O$ reaction for the full-recoil and no-recoil cases. Spectroscopic factors are put equal to one here. The optical-model potential in the incident channel had the form

$$V(r_a) = -(V+iW)f(r_a, R, \delta) - iW_s\left[-4\delta\frac{df(r_a, R', \delta')}{dr_a}\right] + V_C(r_a),$$

$$f(r_a, R, \delta) = \left[1+\exp\left(\frac{r_a - R}{\delta}\right)\right]^{-1},$$

and V_C is the Coulomb potential for a uniformly charged sphere of radius R_C. The optical-model potential in the outgoing channel had the same form. The optical-model parameters which were used are from fits to the elastic scattering data[22,23] and are given in Table III. Reasonable changes in these parameters did not change the general character of the two calculated curves. The calculation of the full-recoil curve was done including the matrix elements of 12 partial waves; this number was found to be sufficient for this energy. All calculations were carried out in double precision with less than 18 000 words of the memory

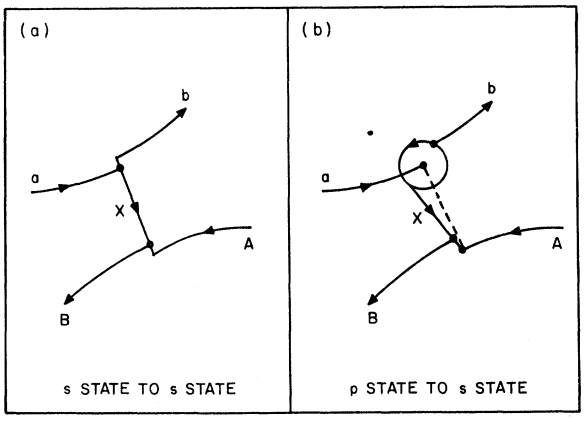

FIG. 7. Schematic diagram of the classical interpretation of form factors for (a) s-state to s-state transfer such as occurs in $^{12}C(^6Li, d)^{16}O$ and (b) p-state to s-state transfer such as occurs in $^{12}C(^7Li, t)^{16}O$ reaction.

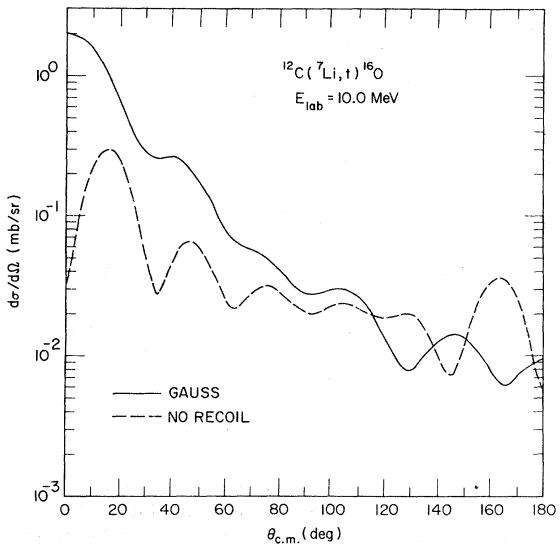

FIG. 8. Differential cross section for the $^{12}C(^7Li, t)^{16}O$ reaction calculated with the full-recoil program GAUSS and calculated with a no-recoil program (Ref. 20). Spectroscopic factors have been put equal to one in both cases.

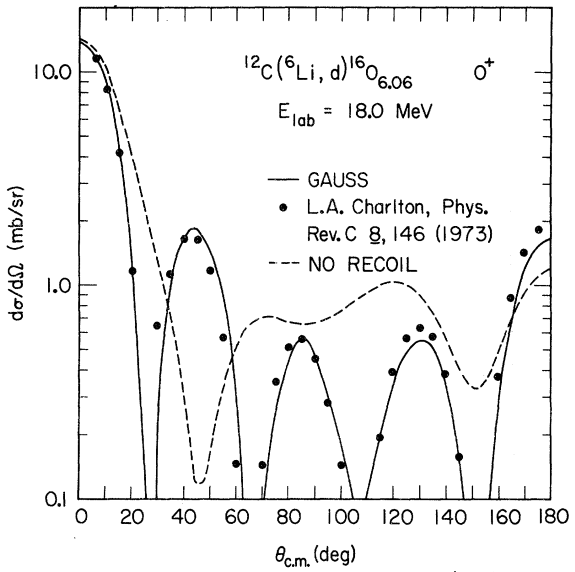

FIG. 9. Differential cross section for the $^{12}C(^6Li, d)^{16}O^*(6.06)$ reaction calculated with full-recoil program GAUSS, with full-recoil program of Refs. 14 and 24, and no-recoil program of Ref. 20. Spectroscopic factors have been put equal to one.

of the University of Iowa's IBM 360/65 computer. The small amount of memory was possible because the Gaussian expansions provided an analytic expression for the form factor.

There are differences in shape as well as magnitude for the full-recoil and no-recoil cases. This is especially true for the forward angles. One is forward peaked and the other is not. This contrasts with results obtained for higher energies with the (^{6}Li, d) reaction where full-recoil and zero-range calculations give essentially the same shape.[11] The contrast is not unexpected in view of the discussion in Sec. III.

Figure 9 shows calculated differential cross sections for the $^{12}C(^6Li, d)^{16}O$(6.06 MeV, 0^+ state) reaction. Full-recoil cases calculated with program GAUSS and calculated by Charlton[14,24] are both shown. In each case the spectroscopic factors are put to one and absolute values are being compared. The two programs are based on rather different approaches so the agreement gives some support to the validity of the program. In the no-recoil case shown in Fig. 9, the calculation gives a forward peak but the rest of the curve is in rather poor agreement with the full-recoil case. Perhaps this disagreement is due to the large transferred-mass to target-mass ratio considered here in contrast to that considered by Strohbusch, Bauer, and Fulbright.[11] The peaking at the most forward angles shown in both the full-recoil and the no-recoil cases is again to be expected on the basis of the discussion in Sec. III.

GAUSS was tested against a number of published results for a varied fare of nuclear reactions. A heavier beam and target were considered in the case of the $^{40}Ca(^{16}O, ^{12}C)^{44}Ti$(g.s.) reaction at 42 MeV. This reaction has previously been considered by De Vries[25] and Blair *et al.*[10] An α particle transfer occurs between spin zero states. As shown in Fig. 10, the present results are in agreement with the earlier results both in magnitude and shape in the region of the broad bump around

TABLE III. Parameters for optical potentials.

	V (MeV)	W (MeV)	W_s (MeV)	R (fm)	δ (fm)	R' (fm)	δ' (fm)	R_C (fm)
$^7Li+^{12}C$ [a]	157.0	0.0	23.5 [b]	3.50	0.650	3.50	0.650	3.50
$t+^{16}O$ [c]	146.8	19.3	0.0	3.53	0.550	3.53	0.550	3.50
$^6Li+^{12}C$ [d]	80.0	0.0	5.0	2.97	0.800	3.43	0.700	4.58
$d+^{16}O^*$ [d]	80.0	0.0	5.0	2.52	0.717	4.00	0.625	3.27

[a] From Ref. 22.
[b] Linear interpolation.
[c] From Ref. 23.
[d] From Ref. 8.

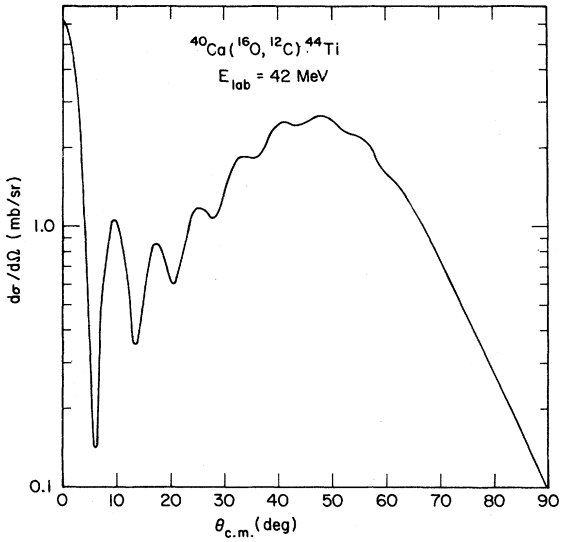

FIG. 10. Differential cross section for the $^{40}Ca(^{16}O, ^{12}C)^{44}Ti$ reaction at 42 MeV calculated with full-recoil program GAUSS. Spectroscopic factors have been put equal to one.

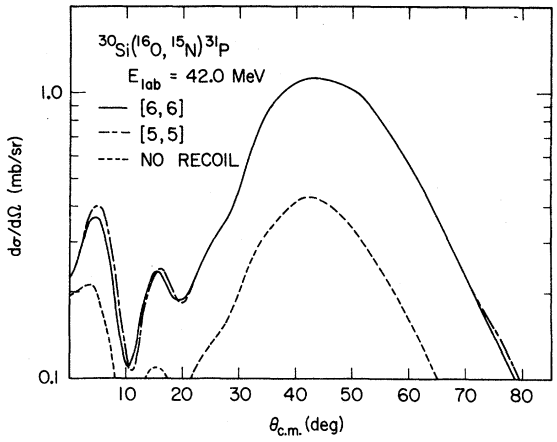

FIG. 11. Differential cross section for the $^{30}Si(^{16}O, ^{15}N)^{31}P$ reaction at 42 MeV calculated with full-recoil program GAUSS. Results with six Gaussians for each expansion [6, 6] and five Gaussians for each expansion [5, 5], are shown. Cross section calculated with no-recoil program of Ref. 20 is also shown. Spectroscopic factors have been put equal to one.

45° but show more oscillation at forward angles. The reason for this difference is not known since input parameters were identical to those used in Ref. 25. In this case, and in all other cases which were considered, integration ranges and step sizes were varied until results were stable and consistent. Running time for such checks was not great since checks on a few matrix elements proved sufficient. Care was taken to ensure that enough Gaussians were used to represent the ^{44}Ti wave function accurately. This wave function has 6 nodes and 17 Gaussians were used in its expansion. The number of Gaussians was varied and had no significant affect on the forward oscillations.

Results of calculations with GAUSS are shown in Fig. 11 for the single-proton transfer reaction $^{30}Si(^{16}O, ^{15}N)^{31}P$ at 42 MeV. Results are shown for two different choices of numbers of Gaussians used for $\varphi(r_{Ax})$ and $V(r_{bx})\varphi(r_{bx})$; six each in one case and five each in the other. The bound states in this reaction are simpler than those occurring in the preceding α transfer reaction and, consequently, a smaller number of Gaussians is adequate. Differences arising from the different number of Gaussians only appear forward of 20°. Calculations for higher bombarding energies were carried out with an appropriate increase in the number of partial waves considered. The absolute value of the cross section at 45° (1.232 mb/sr) is in excellent agreement with that given by Blair *et al.*[10] (1.256 mb/sr). The no-recoil calculation shows excellent agreement in shape with the full-recoil calculation in this case, which is to be expected for a light-mass transfer.

GAUSS and LOLA[26] were both used to calculate the differential cross section for the $^{11}B(^{3}He, ^{7}Be)^{7}Li$ reaction which is the suggested test case for LOLA. LOLA is a full-recoil program with a different ap-

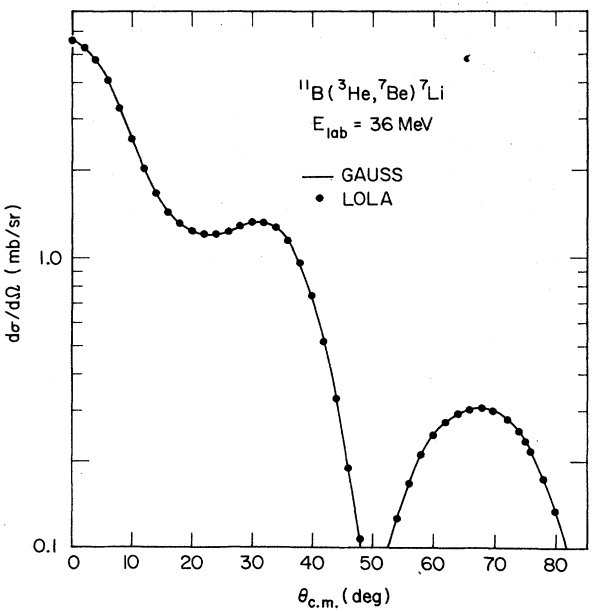

FIG. 12. Differential cross section for the $^{11}B(^{3}He, ^{7}Be)^{7}Li$ reaction at 36 MeV calculated with full-recoil programs GAUSS and LOLA. Spectroscopic factors have been put equal to one.

proach toward the calculation than that used in GAUSS. Identical input parameters were used, of course, in both calculations. The calculations with LOLA could not be fitted into the University of Iowa's IBM 360/65 computer so they were run for us at the Argonne National Laboratory. GAUSS has been run in both places. Excellent agreement was found for this test case as can be seen in Fig. 12.

In summary, Gaussian expansions of the bound-state wave functions and the interaction potential simplify the DWBA calculations and make it easier to interpret the form factor. These simplifications have made possible the construction of a computer code (GAUSS) which requires no more than 18 000 words of memory to carry out the exact DWBA calculation.

ACKNOWLEDGMENTS

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