Effect of Approximate Wave Functions in Composite-Particle Scattering*

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Many investigators have studied the scattering of low-energy nucleons by light nuclei using a single-particle effective potential which is derived from a many-nucleon Hamiltonian under the assumption that the contribution to the scattering by virtual excitations of the target nucleus can be neglected. In addition, they have approximated the ground-state wave functions of the target nuclei by crude variational wave functions, thus introducing an unknown error into the results of the scattering calculation. In this paper we investigate that error for the specific case of neutron-triton scattering. To do this we derive three approximate effective potentials which differ from each other and from the exact single-particle effective potential by the same order in the error of the approximate triton wave function. The difference between the phase shifts calculated with the approximate potentials gives an indication of the uncertainty in the calculations, and as the approximate triton wave function is improved the difference decreases. Our work shows that previous calculations involve large errors which may be reduced by improving the approximate target wave function.

I. INTRODUCTION

The complexity of the nucleon-nucleon interaction and the difficulties of the many-body problem require the construction of simplified models to describe nuclear reactions. One model used for the description of the scattering of nucleons from light nuclei is the resonating-group-structure method.¹⁻³ In this method the low-energy elastic scattering states of the nucleon-nucleus system are approximated by functions ψ , of the form

$$\psi = A\varphi F, \qquad (I.1)$$

where φ is the ground-state eigenfunction of the Hamiltonian for the target nucleus, F is the wave function of the nucleon, and A is the operator which properly antisymmetrizes the wave function. Equation (I.1) is known as the no-polarization approximation, because all virtual excited states of the nucleus have been neglected.

If the nuclear wave function φ were known, the wave function ψ could be used in the Schrödinger equation of the nucleon-nucleus system to derive an effective single-particle nonlocal potential which gives the correct phase shifts for the nopolarization approximation. Then, these phase shifts could be compared with the experimental phase shifts, and conclusions could be drawn about the validity of the no-polarization approximation, the structure of the target nucleus, or the appropriateness of the particular parameters of the two-nucleon interaction.

In practice, though, φ is not known; instead, an approximate wave function for the target nucleus is found by using the Ritz variational principle. The nucleon-nucleus effective potential is then derived using the variational wave function, and the results of scattering calculations with this potential are used for the comparison with experiment. In previous calculations conclusions have been drawn without considering the size of the error introduced by using a variational wave function for the target in the scattering calculations. The purpose of the present work is to investigate the size of the error this approximation introduces into the scattering calculation.

We consider the specific case of neutron-triton scattering using the RGSM. This means that we accept the no-polarization approximation and the two-nucleon potential as basic assumptions of this work. Our goal here is not detailed agreement with experiment, but an understanding of a source of uncertainty in the calculation of the phase shifts for scattering processes with composite particles.

In the next section we give three forms for an effective nucleon-nucleus potential which are functionals of the target ground-state wave function, and which would be equivalent if the exact target wave function were used. The differences in the phase shifts calculated with the different forms give an indication of the uncertainty caused by the use of the variational wave function.

In Sec. III a number of approximate triton wave functions are constructed and lower bounds are found on their overlap with the ground state of the model triton Hamiltonian. Next, phase shifts for neutron-triton elastic scattering are calculated using these triton wave functions. We find that as the lower bound to the overlap of the approximate wave function with the true eigenfunction is increased, the phase shifts change appreciably.

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When a simple triton wave function of the form used in previous RGSM calculations is used, the uncertainty indicated by the difference between the phase shifts calculated with the different effective potentials is comparable with the present experimental uncertainty. This shows that the approximate forms used for the ground-state wave function in previous RGSM calculations are not sufficiently accurate to allow a definitive comparison of the model with the experiment.

Finally, in the Conclusions, we discuss the possibilities for further investigation of this problem, and point out the relevance of our work to other models of nuclear reactions.

II. STRUCTURE OF EFFECTIVE POTENTIALS

For neutron-triton scattering in the no-polarization approximation⁴ the wave function ψ_{n-T} of the system is given by a product of the model triton ground-state wave function, φ_T , and F_n , the wave function of the incoming neutron, i.e.,

$$\psi_{n-T} = A \varphi_T F_n, \qquad (II.1)$$

where A is the antisymmetrization operator.

In order to calculate the neutron-triton scattering in the no-polarization approximation, the ground-state wave function φ_T must be known. By definition φ_T is the eigenfunction of the triton model Hamiltonian H_T , satisfying

$$H_T \varphi_T = E_T \varphi_T, \qquad (II.2)$$

where E_T is the model triton binding energy.

The Hamiltonian H of the neutron-triton system can be written as

$$H = H_T + H_{n-T} , \qquad (II.3)$$

where H_{n-T} is the kinetic energy of the neutron plus its interaction with the triton. The Schrödinger equation in the no-polarization approximation for the neutron-triton system is

$$(H_T + H_{n-T})A\varphi_T F_n = (E_T + E_n)A\varphi_T F_n, \qquad (II.4)$$

where E_n is the energy of the neutron. Equation (II.4) for the neutron scattering amplitude F_n may be reduced to a single-particle equation with a nonlocal potential by multiplying by φ_T from the left and integrating over the triton coordinates τ_T .⁵ This gives

$$\int d\tau_T \varphi_T [(H_T + H_{n-T}) - (E_n + E_T)] A \varphi_T F_n = 0.$$
(II.5)

Before proceeding to examine Eq. (II.5) further, we introduce a notation which allows us to see the effects of antisymmetrization more clearly. Let the indices 1, 2, and 4 stand for neutrons and 3 for the proton. Then in the center-of-mass coordinates the properly antisymmetrized wave function of the neutron-triton system may be written

$$\Psi(1234) = \sqrt{\frac{1}{6}} \left[\varphi_T(123) F_n(123-4) - \varphi_T(432) F_n(432-1) \right]$$

$$-\varphi_{T}(143)F_{n}(143-2)], \qquad (II.6)$$

where, for example, the term

$$\varphi_T(423)F_n(423-1)$$
 (II.7)

means that the triton wave function depends upon the spin-space coordinates of neutrons 4 and 2, as well as those of the proton, while the neutron scattering amplitude is a function of the spin of neutrons 1 and its position relative to the center of mass of particles 4, 2, and 3.

In the center-of-mass system the Hamiltonian H of the four particles may be written as

$$H = H_{ijk} + H_{ijk-1}, \qquad (II.8)$$

where H_{ijk} is the Hamiltonian of the triton, and H_{ijk-1} is the kinetic energy operator for the scattered neutron plus the interaction of the neutron with the nucleons of the triton. We may express H_{ijk} as

$$H_{ijk} = T_{ij} + T_{ij-k} + V_{ij} + V_{ik} + V_{jk}, \qquad (II.9)$$

with T_{ij} the kinetic energy operator of particles i and j in their center of mass, and T_{ij-k} the kinetic energy operator of particle k relative to the center of mass of particles i and j. The potential between particles i and j is given by V_{ij} . The motion of nucleon l relative to the triton is given by

$$H_{ijk-l} = T_{ijk-l} + V_{il} + V_{jl} + V_{kl}, \qquad (II.10)$$

where T_{ijk-l} is the kinetic energy operator of particle *l* relative to the center of mass of particles *i*, *j*, and *k*. From Eq. (II.8) for *H*, it is clear that we may write

$$H = \frac{1}{2} \left[H_{123} + H_{123-4} + H_{423} + H_{423-1} \right].$$
 (II.11)

This form of the Hamiltonian, which is obviously symmetric under the exchange of particles 1 and 4, insures that the effective potential will be Hermitean.

Using the above notation we rewrite Eq. (II.5) as

$$\int d\tau_{123} \varphi_T (123) [H_{123} + H_{123-4} - (E_T + E_n)] \varphi_T (123) F_n (123-4) \\ - \int d\tau_{123} \varphi_T (123) [H_{123} + H_{123-4} + H_{423} + H_{423-1} - 2(E_T + E_n)] \varphi_T (423) F_n (423-1) = 0.$$
(II.12)

We have used the antisymmetry of $\varphi(ij3)$ under the exchange of neutrons *i* and *j* to simplify the second line of Eq. (II.12).

It is possible, of course, to form other equally valid equations for $F_n(123-4)$ which give the same result as Eq. (II.12). If we use the property

$$H_{ij3}\varphi(ij3) = E_T\varphi(ij3) \tag{II.13}$$

in Eq. (II.12) the result is

$$\int d\tau_{123}\varphi_T(123)[H_{123-4} - E_n]\varphi_T(123)F_n(123-4) - \int d\tau_{123}\varphi_T(123)[H_{123-4} + H_{423-1} - 2E_n]\varphi_T(423)F_n(423-1) = 0.$$
(II.14)

Equation (II.14) is an exact equation for the neutron scattering amplitude which we may write in more detail by using the definitions

 $H_{123-4} = T_{123-4} + V_{14} + V_{24} + V_{34}$ (II.15)

and

$$H_{423-1} = T_{423-1} + V_{14} + V_{12} + V_{13} . (II.16)$$

But, we may write

$$T_{123-4} = \frac{1}{8} T_{23-1} + \frac{9}{8} T_{23-4} + \frac{9}{16m} \vec{p}_{23-1} \cdot \vec{p}_{23-4}$$
(II.17)

and

$$T_{423-1} = \frac{9}{8}T_{23-1} + \frac{1}{8}T_{23-4} + \frac{9}{16m}\vec{p}_{23-1} \cdot \vec{p}_{23-4}, \qquad (II.18)$$

where m is the mass of the nucleon and \vec{p}_{ij-k} is the momentum of particle k relative to the center of mass of particles i and j. Using Eqs. (II.15)-(II.18), Eq. (II.14) becomes

$$\int d\tau_{123} \varphi_T (123) [H_{123-4} - E_n] \varphi_T (123) F_n (123-4) - \int d\tau_{123} \varphi_T (123) \left(\frac{5}{4} T_{23-1} + \frac{5}{4} T_{23-4} + \frac{9}{8m} \tilde{p}_{23-1} \cdot \tilde{p}_{23-4} + V_{12} + V_{13} + 2V_{14} + V_{24} + V_{34} - 2E_n \right) \varphi_T (423) F_n (423-1) = 0.$$
(II.19)

Part of our investigations will be based upon Eq. (II.19).

Yet another exact equation, which has been used in previous work, may be formed from Eq. (II.19). The property that $\varphi(ijk)$ is the eigenstate of the triton Hamiltonian, that is,

$$H_{ijk}\varphi_T(ijk) = E_T\varphi_T(ijk), \qquad (II.20)$$

may be used again, as

$$T_{23-1}\varphi_T(123) = (-T_{23} - V_{12} - V_{13} - V_{23} + E_T)\varphi_T(123)$$
(II.21)

and

$$T_{23-4}\varphi_T(423) = (-T_{23} - V_{23} - V_{24} - V_{34} + E_T)\varphi_T(423).$$
(II.22)

If Eqs. (II.21) and (II.22) are substituted in Eq. (II.19) one obtains

$$\int d\tau_{123} \varphi_T (123) [H_{123-4} - E_n] \varphi_T (123) F_n (123-4) - \int d\tau_{123} \varphi_T (123) \left(-\frac{5}{2} T_{23} - \frac{1}{4} V_{12} - \frac{1}{4} V_{13} + 2V_{14} + \frac{9}{8m} \vec{p}_{23-1} \cdot \vec{p}_{23-4} - \frac{5}{2} V_{23} - \frac{1}{4} V_{24} - \frac{1}{4} V_{34} + \frac{5}{2} E_T - 2E_n \right) \varphi_T (423) F_n (423-1) = 0.$$
(II.23)

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Equation (II.23), which we have derived at some length, and Eq. (II.12) are equations for F(123-4) in the no-polarization approximation which have provided the basis for previous calculations of neutron-triton scattering.^{6,7} For this reason we chose them, along with Eq. (II.19), for further investigation.

Equation (II.19) depends upon the triton wave function φ_T , while Eqs. (II.12) and (II.23) depend upon both φ_{T} and the binding energy E_{T} . Even with the simple triton Hamiltonian used in the RGSM it is very difficult to find the exact ground-state wave function φ_T and eigenvalue $E_{T^{*8}}$ In fact, the exact wave function φ_T would probably not be useful for the scattering calculation, because it is likely to be too complex. This is true of very good approximate wave functions, as we discuss in Sec. IV. For this reason, an approximate triton groundstate wave function Φ_T with a form convenient for the scattering calculation, and its upper bound E_{η} to the binding energy are found. The correction term Φ'_{T} to the approximate wave function Φ_{T} is defined by the relation,

$$\varphi_T = Z^{1/2} (\Phi_T + \Phi_T') , \qquad (II.24)$$

where Φ_T' is orthogonal to Φ_T . Because both φ_T

and
$$\Phi_{\tau}$$
 are normalized to 1, the factor $Z^{1/2}$ is

$$Z^{1/2} = \langle \varphi_T | \Phi_T \rangle \leq 1.$$
 (II.25)

It follows that

$$1 = \langle \varphi_T | \varphi_T \rangle = Z(1 + \| \Phi'_T \|^2), \quad (II.26)$$
 or

$$\|\Phi_{r}'\|^{2} = (1/Z) - 1.$$
 (II.27)

As Z approaches 1, Φ'_T diminishes and the approximate wave function Φ_T approaches the eigenstate φ_T . Using the overlap we can investigate the effect on the results of calculating neutron-triton scattering with an approximate bound-state wave function.

To form equations for $F_n(123-4)$ which depend explicitly upon the approximate triton wave function Φ_T we first substitute the relation

$$\varphi_{T}(ijk) = Z^{1/2} [\Phi_{T}(ijk) + \Phi_{T}'(ijk)]$$
(II.28)

in Eqs. (II.12), (II.19), and (II.23), and use the facts that $\label{eq:interm}$

$$Z \approx 1 - \|\Phi_T^{\prime}\|^2 \approx 1 \tag{II.29}$$
 and

$$E_{T} = E_{H} + O(\|\Phi_{T}'\|^{2}) \approx E_{H}.$$
(II.30)

For Eq. (II.12) this gives

$$\int d\tau_{123} [\Phi_T(123) + \Phi_T'(123)] [H_{123} + H_{123-4} - (E_U + E_n)] [\Phi_T(123) + \Phi_T'(123)] F_n(123-4) \\ - \int d\tau_{123} [\Phi_T(123) + \Phi_T'(123)] [H_{123} + H_{123-4} + H_{423} + H_{423-1} - 2(E_U + E_n)] [\Phi_T(423) + \Phi_T'(423)] F_n(423-1) = 0.$$
(II.31)

From Eq. (II.19) we find

$$\int d\tau_{123} [\Phi_{T}(123) + \Phi_{T}'(123)] [H_{123-4} - E_{n}] [\Phi_{T}(123) + \Phi_{T}'(123)] F_{n}(123-4) - \int d\tau_{123} [\Phi_{T}(123) + \Phi_{T}'(123)] \left(\frac{5}{4}T_{23-1} + \frac{5}{4}T_{23-4} + \frac{9}{8m}\vec{p}_{23-1} \cdot \vec{p}_{23-4} + V_{12} + V_{13} + 2V_{14} + V_{24} + V_{34} - 2E_{n}\right) \times [\Phi_{T}(423) + \Phi_{T}'(423)] F_{n}(423-1) = 0, \qquad (II.32)$$

and Eq. (II.23) becomes

$$\int d\tau_{123} [\Phi_T(123) + \Phi_T'(123)] [H_{123-4} - E_n] [\Phi_T(123) + \Phi_T'(123)] F_n(123-4) - \int d\tau_{123} [\Phi_T(123) + \Phi_T'(123)] \left(-\frac{5}{2} T_{23} - \frac{1}{4} V_{12} - \frac{1}{4} V_{13} + 2V_{14} + \frac{9}{8m} \vec{p}_{23-1} \cdot \vec{p}_{23-4} + \frac{5}{2} E_U - \frac{1}{4} V_{24} - \frac{1}{4} V_{34} - 2E_n \right) \\ \times [\Phi_T(423) + \Phi_T'(423)] F_n(423-1) = 0.$$
(II.33)

If in Eqs. (II.31), (II.32), and (II.33) terms of order Φ'_T or higher are neglected, the result will be three approximate equations for the neutron wave function F(123-4) which depend only upon Φ_T and E_U . For brevity we shall refer to them as approximations I, II, and III, respectively. Approximations I and III depend upon both Φ_T and E_U , while approximation II depends only upon Φ_T .

By comparing Eqs. (II.31)-(II.33) it is clear that for each of the approximations the dominant correction term is of the first order in Φ'_r . Thus, we have no reason to prefer one approximation 2160

rather than another. From these equations and their derivations, it is clear that as the triton variational wave function is improved, that is, as Φ'_T tends to zero, the three approximations tend to exact equations for F(123-4). The difference between the phase shifts calculated with the approximations thus gives an indication of their error with respect to the exact phase shift.

Before we can investigate neutron-triton scattering numerically, we must first select a twonucleon potential, construct triton variational wave functions, and calculate the three approximate effective potentials in detail. We do this in the next section.

III. TWO-NUCLEON POTENTIAL AND APPROXIMATE TRITON WAVE FUNCTION

It is well known that it is possible to fit the twonucleon data for energies below about 10 MeV using a potential with a simple radial form.⁹ Previous workers^{2, 6, 7} have found that a Gaussian form is particularly convenient for the calculation of nucleon-nucleus scattering, so we have chosen a two-nucleon potential V_{ij} with space-exchange operator M_{ij} of the form

$$V_{ij} = (w + mM_{ij})V_0 e^{-\mu r_{ij}^2}, \qquad (\text{III.1})$$

where the constants w, m, V_0 , μ have the values

$$w = m = 0.5$$
,
 $V_0 = -51.1 \text{ MeV}$,
 $\mu = 0.39 \text{ F}^{-2}$. (III.2)

This potential, which is spin independent, has been used in a determination of very good bounds¹⁰ on the binding energy of our model triton Hamiltonian, which will prove useful in this investigation.

The parameters for the approximate solutions Φ_t (123) of the triton Schrödinger equation may be found from the Ritz variational principle by minimizing the upper bound to the triton binding energy E_U , given by,

$$E_{U} = \int d\tau_{123} \Phi_{T}(123) H_{123} \Phi_{T}(123) \,. \tag{III.3}$$

To apply the Ritz method to the triton ground state, the trial functions $\Phi_T(123)$ must be constructed from suitable spatial and spin functions. This spin-space structure is determined by the Pauli principle and the characteristics of the two-nucleon potential used for the calculation.

When a spin-independent central potential is used, the ground state is purely a spatially symmetric *S* state. So, to form a correctly antisymmetrized trial wave function, the spatially symmetric *S* state is coupled to a spinor made up of the three nucleon spinors coupled to $S_T = \frac{1}{2}$. This gives $J = \frac{1}{2}$, the total angular momentum of the triton. We shall denote the triton trial function by $\Phi_T(123)$, and the space part of that wave function by $\Phi(123)$. Then

$$\Phi_{\tau}(123) = \Phi(123)\chi(123), \qquad (III.4)$$

where $\chi(123)$ is the three-particle spinor. In terms of the neutron spinors S_1 , S_2 , and the proton spinor S_3 , $\chi(123)$ is given by

$$\chi(123) = [(S_1, S_2)_0, S_3]_{S_T}^{m_T}.$$
 (III.5)

Equation (III.5) means that the neutron spinors are coupled to spin zero, and then the proton spinor or is coupled to the spinor of the neutrons. This gives the triton spinor of spin $S_T = \frac{1}{2}$ with z component M_T .

A spatial trial function used in earlier calculations of neutron-triton scattering^{6,7} is

$$\Phi(123) = N_S \exp\left[-\frac{1}{2}\alpha(r_{12}^2 + r_{13}^2 + r_{23}^2)\right], \qquad \text{(III.6)}$$

which was selected because of its convenience for the scattering calculation and not because it gives a good upper bound to the triton binding energy. The upper bound to the triton binding energy can be improved while retaining the convenience of Gaussians by using the trial function

$$\Phi(123) = N'_{S} \left\{ \exp\left[-\frac{1}{2}\lambda(r_{12}^{2} + r_{13}^{2} + r_{23}^{2})\right] + x \exp\left[-\frac{1}{2}\nu(r_{12}^{2} + r_{13}^{2} + r_{23}^{2})\right] \right\},$$
(III.7)

and further improvement may be obtained by using

$$\begin{split} \Phi(\mathbf{123}) &= N_S'' \left\{ \exp\left[-\frac{1}{2}\beta(r_{12}^2+r_{13}^2+r_{23}^2)\right] \right. \\ &+ y \exp\left[-\frac{1}{2}\gamma(r_{12}^2+r_{13}^2+r_{23}^2)\right] \\ &+ z \exp\left[-\frac{1}{2}\delta(r_{12}^2+r_{13}^2+r_{23}^2)\right] \right\}, \end{split}$$

(III.8)

where N_s , N'_s , N''_s are normalization factors, and α , λ , ν , β , γ , δ , x, y, and z are the variational parameters.

In Table I, we give the values of the variational parameters and the upper bounds¹¹ E_{U} to the total triton ground-state energies E_{T} . As may be seen from the table, increasing the number of parameters lowers E_{U} , that is, moves it closer to E_{T} , the true eigenvalue.

Next, we wish to know the overlap of the approximate wave function Φ_T with the eigenstate φ_T . Because φ_T is unknown, we cannot find the overlap directly. However, a lower bound to the overlap $\langle \varphi_T | \Phi_T \rangle$ has been derived¹⁰ in terms of E_U , E_1 (the energy of the first excited state of H_T), and E_T or E_L (a lower bound to E_T). It can be shown that

TABLE I. Parameters of the triton variational wave functions.

One Gaussian	$E_{U} = -6.89 \text{ MeV}$	$\alpha = 0.202 \ {\rm F}^{-2}$				
Two Gaussians	$E_{U} = -9.07 { m MeV}$	$\lambda = 0.105 \text{ F}^{-2}$	x = 5.03	$\nu = 0.349 \text{ F}^{-2}$		
Three Gaussians	$E_U = -9.16 \text{ MeV}$	$\beta = 0.145 \ { m F}^{-2}$	y = 2.92	$\gamma = 0.406 \ {\rm F}^{-2}$	z = 0.062	$\delta = 0.047$

$$1 \geq \langle \varphi_T | \Phi_T \rangle \geq \left(\frac{E_1 - E_U}{E_1 - E_T} \right)^{1/2} \geq \left(\frac{E_1 - E_U}{E_1 - E_L} \right)^{1/2} .$$
(III.9)

For the triton model considered here we assume that there are no three-body bound excited states; then E_1 is the two-body binding energy with the third particle free. Since the eigenvalue E_T is not known, the expression with E_L must be used to estimate the overlap.

One method widely used¹² to find lower bounds requires a trial function $\Psi(P_i)$. Defining

$$\langle H_T \rangle \equiv \int d\tau \Psi^*(P_i) H_T \Psi(P_i)$$
 (III.10)

and

$$\langle H_T^2 \rangle \equiv \int d\tau \Psi^*(P_i) H_T^2 \Psi(P_i),$$

it has been shown that¹²

$$E_T \ge E_L = \langle H_T \rangle - \frac{\langle H_T^2 \rangle - \langle H_T \rangle^2}{E_1 - \langle H_T \rangle} , \qquad (\text{III.11})$$

which is known as Temple's formula.¹² This expression for E_L is a function of the trial-wavefunction parameters, which are varied until the maximum value of E_L is found. Then using E_L the overlap $\langle \varphi_T | \Phi_T \rangle$ may be found. Unfortunately, as has been demonstrated in many calculations in both $atomic^{12}$ and $nuclear^{10}$ physics, lower bounds tend to lie much further from the eigenvalue than do upper bounds found with the same trial wave function. Therefore, to obtain a good lower bound one must use very complex trial wave functions. This problem has been studied for our potential by Herndon and Tang,¹⁰ with trial functions of an elaborate functional form that did not permit an analytic evaluation of expression for E_{II} and $E_{I.}$. Instead, it was necessary to find E_{II} and E_L numerically, using Monte-Carlo methods to evaluate multidimensional integrals. The result of their calculation is,

$$E_{\rm U} = -9.75 \pm 0.04 \,\,{\rm MeV}$$
, (III.12)

and

$$E_L = -9.99 \pm 0.05 \text{ MeV}$$
.

We will use this value of E_L in Eq. (III.11) to get lower bounds on the overlap of the variational and exact wave functions.

The results, using the lower bound of Eq. (III.12), are

	(III.13)
$Z^{1/2} = \left\langle \Phi_T \left \varphi_T \right\rangle_3 \ge 0.955 \right.$	for the three-Gaussian Φ_{T} .
$Z^{1/2} = \left\langle \Phi_T \left \varphi_T \right\rangle_2 \ge 0.951 \right.$	for the two-Gaussian Φ_{T} ,
$Z^{1/2} = \langle \Phi_T \varphi_T \rangle_1 \ge 0.822$	for the one-Gaussian Φ_T ,

The lower bound to the overlap of our trial wave function Ψ_T with the eigenfunction φ_T may be improved by using a relation given by Weinhold.¹³ Let Ψ_T be a trial wave function which has the overlap $\langle \Psi_T | \varphi_T \rangle$ with φ_T , then

$$Z^{1/2} \geq \langle \Phi_T | \Psi_T \rangle \langle \Psi_T | \varphi_T \rangle - [(1 - \langle \Phi_T | \Psi_T \rangle^2)(1 - \langle \Psi_T | \varphi_T \rangle^2]^{1/2},$$
(III.14)

where $\langle \Phi_T | \Psi_T \rangle$ is the overlap of the trial wave functions Φ_T and Ψ_T . If the overlap $\langle \Psi_T | \varphi_T \rangle$ is near unity, Eq. (III.14) gives a lower bound to $Z^{1/2}$ which is near the actual value. However, the overlap $\langle \Psi_T | \varphi_T \rangle$ cannot be calculated, but a lower bound $S^{1/2}$ to the overlap can be found from Eq. (III.9). Then, from Eq. (III.14) it follows that

$$Z^{1/2} \ge S^{1/2} \langle \Phi_{\mathbf{r}} | \Psi_{\mathbf{r}} \rangle . \tag{III.15}$$

The trial wave functions Ψ_T given in Ref. 10 cannot be used to calculate the overlap $\langle \Phi_T | \Psi_T \rangle$ conveniently; therefore, we use the trial wave function Ψ_T of the form,

$$\Psi_{T} = \sum_{l, m, n} a_{l m n} s^{l-1} t^{m-1} u^{n-1} e^{-(\alpha s + \beta u)}, \qquad \text{(III.16)}$$

where $s = r_{13} + r_{23}$, $l = r_{13} - r_{23}$, $u = r_{12}$, and the sum is terminated by the condition $l + m + n \le N$. Only odd values of *m* are retained in the summation, since we require the wave function to be spatially symmetric under the interchange of particles 1 and 2. Using a program written by L. Schlessinger the coefficients a_{lmn} and the upper bound to the binding energy can be calculated very quickly on an IBM 360/65 computer. For *N* equal to 10 the calculations required less than 23 sec, with the result for the upper bound to the ground-state energy,

$$E_{U} = \langle \Psi_{T} | H_{T} | \Psi_{T} \rangle = -9.79 \text{ MeV}. \qquad (\text{III.17})$$

Using the lower bound to the energy given in (III.12) one finds

$$\langle \Psi_T | \varphi_T \rangle \ge 0.989$$
 (III.18)

(III.20)

The actual overlap of Ψ_T with φ_T is probably much better than this; however, a better lower bound to the energy is required before we can improve the result given above.

The overlap of our approximate wave functions with Ψ_T are:

$$\begin{split} \langle \Phi_T | \Psi_T \rangle_1 &= 0.959 , & \text{for one Gaussian,} \\ \langle \Phi_T | \Psi_T \rangle_2 &= 0.992 , & \text{for two Gaussians,} \\ \langle \Phi_T | \Psi_T \rangle_3 &= 0.995 , & \text{for three Gaussians.} \end{split}$$
(III.19)

Using these values in (III.16) we find

 $Z^{1/2} \ge 0.948$, for one Gaussian, $Z^{1/2} \ge 0.981$, for two Gaussians, $Z^{1/2} \ge 0.984$, for three Gaussians.

It is likely that the actual value of $Z^{1/2}$ is even

TABLE II. Calculated phase shifts for one-Gaussian (1G), two-Gaussian (2G), and three-Gaussian (3G) triton trial wave functions. All energies are neutron laboratory energies.

	1 MeV	2.5 MeV	5 MeV	8 MeV	14 MeV	
	S-wave phase shifts in degrees.					
	Approximation I					
$1\mathrm{G}$	-26.6	-41.7	-58.2	-72.4	-92.9	
$2\mathrm{G}$	-29.2	-45.5	-62.6	-77.0	-96.8	
3G	-28.9	-45.4	-63.8	-78.1	-98.2	
	Approximation II					
1G	-23.5	-37.0	-52.1	-65.4	-85.5	
2G	-28.8	-42.1	-59.0	-73.6	-94.7	
3G	-27.9	-43.9	-61.5	-76.3	-96.6	
	Approximation III					
1G	-16.8	-27.6	-40.8	-53.7	-74.6	
2G	-23.1	-37.3	-53.9	-69.1	-92.1	
3G	-26.6	-42.1	-59.2	-73.9	-94.4	
	<i>P</i> -wave phase shifts in degrees					
	Approximation I					
1G	1.4	4.9	10.4	14.3	15.2	
2G	1.9	6.0	11.3	13.9	12.9	
3G	1.6	5.5	11.2	14.2	12.9	
	Approximation II					
$1\mathrm{G}$	0.4	1.3	3.2	5.4	8.1	
2G	0.9	3.3	7.2	10.4	12.0	
3G	1.1	4.0	8.7	11.8	11.7	
		App	roximatio	on III		
$1\mathrm{G}$	-0.6	-2.0	-3.7	-4.4	-1.5	
2G	-0.1	0.2	2.3	6.0	10.8	
3G	0.6	2.4	5.9	8.8	10.1	

higher, since the maximum value one can obtain using (III.15) and (III.18) is 0.989.

Given the approximate triton eigenfunction $\Phi(123)$ the wave function $\Psi(1234)$ of the neutron triton system may be written

$$\Psi(1234) = \frac{1}{6}(1 - P_{14} - P_{24})\Phi(123)F_s(r_{123-4})\chi_{1234},$$
(III.21)

where P_{ij} exchanges the spin-space coordinates of neutrons *i* and *j*, and the spinor χ_{1234} , which is defined by

$$\chi_{1234} \equiv \{ [(S_1, S_2)_0, S_3]_{ST}, S_4 \}_{S}^{M_S}, \qquad (\text{III.22})$$

is formed by coupling the triton spinor $[(S_1, S_2)_0, S_3]_{S_T}^{M_T}$ to the spinor S_4 of the scattered neutron to give total spin S (S = 0 or S = 1).

When the two-nucleon potential of Eq. (III.1) and the wave function $\Psi(1234)$ of Eq. (III.16) are used in approximations I-III, there results, after some straight-forward calculation, an integrodifferential equation for the neutron wave function $F_s(\vec{r}_{123-4})$ of the form

$$\begin{aligned} (\nabla_{123-4}^2 + k^2) F_s(\mathbf{\tilde{r}}_{123-4}) &= U(\mathbf{\tilde{r}}_{123-4}) F_s(\mathbf{\tilde{r}}_{123-4}) \\ &+ \int K(\mathbf{\tilde{r}}_{234-1}, \mathbf{\tilde{r}}_{123-4}) F_s(\mathbf{\tilde{r}}_{234-1}) d\mathbf{\tilde{r}}_{234-1}, \end{aligned}$$
(III.23)

where $k^2 = \frac{3}{2} (m/\hbar) E_n$. The local potential $U(\vec{\mathbf{r}}_{123-4})$ is the same for the three approximations, but the kernel $K(\vec{\mathbf{r}}_{234-1}, \vec{\mathbf{r}}_{123-4})$, which arises because of the antisymmetrization of the wave function (III.21) and the space-exchange operator in the two-nucleon potential, is different for each approximation. Since this equation is quite lengthy, it is not given in detail here, but is given in the Appendix. Equation (III.23) may be resolved into partial waves, then solved by a straightforward technique, which is standard for RGSM calculations.¹⁴ We have done this for the various approximate triton model wave functions of Table I for the S and P waves. Our results are discussed in the next section.

IV. NUMERICAL RESULTS AND DISCUSSION

The neutron-triton scattering phase shifts were calculated numerically in order to study their change as the triton variational wave function is improved. Our calculations were performed at five energies up to a neutron lab energy of 14 MeV,¹⁵ for the potential given in Eq. (III.1). The results are given in Table II and Figs. 1 and 2.

In Sec. II it was pointed out that calculations with approximations I-III will give the same results if the exact triton wave function is used. It follows that as we improve the triton approximate wave function, the differences between the phase shifts calculated with the three approximations should decrease. This expectation is confirmed, as illustrated by Figs. 1 and 2 where we show the S- and P-wave shifts.

We showed in Sec. III that there was a considerable improvement in the binding energy and lower bound to the overlap when the triton trial wave function was changed from one to two Gaussians. This improvement is reflected in the phase-shift curves of Figs. 1 and 2, where the difference between the phase shifts calculated with the different approximations is less for the two-Gaussian than for the one-Gaussian triton wave functions.

The binding energy and lower bound to the overlap of the three-Gaussian trial function showed a slight improvement over that of the two-Gaussian wave function. The differences between the phase shifts calculated with the three approximations correspondingly decreased slightly for the three-Gaussian wave functions.

It was stated in Sec. II that the differences between the phase shifts calculated with approximations I, II, or III gives an indication of the uncertainty in the results. By comparing these differences for the S and P waves, it is clear that the P waves have a greater degree of uncertainty than the S waves. In the P waves the centrifugal barrier prevents the neutron from approaching the triton too closely. This means that the tail of the triton wave function is more important in the P waves than in the S waves. It is well known that

variational wave functions can give good values of energy and have totally incorrect asymptotic behavior.¹⁶ It is clear, in fact, that the asymptotic behavior of our variational wave functions is incorrect. As any one of the nucleons moves far away from the other two, the triton wave function should be proportional to $e^{-\kappa r}$, where κ is a constant, and r is the position of the distant nucleon with respect to the center of mass of the other two. But our trial wave functions are proportional to $e^{-\lambda r^2}$ which means that they ultimately drop off too quickly. Thus, there is no reason to believe that as we increase the lower bound to the overlap by improving the binding energy the overlap of all regions of the approximate triton wave function with the true wave function are equally improved. Since the effect of such regions is different in the different approximations, this would account for the greater uncertainty of the P waves.

The characteristics of variational calculations are also probably responsible for another feature of Figs. 1 and 2. Approximation III appears to be somewhat less stable than approximations I and II. That is, approximation III changes more than approximation I or II when the trial wave function is improved from one to two Gaussians, and from two to three. Recall that in deriving approximation II we first used the property of the eigenstate φ_T ,

 $H_T \varphi_T = E_T \varphi_T$,

$$\begin{array}{c} 0^{\circ} \\ -10^{\circ} \\ 20^{\circ} \\ -20^{\circ} \\ -2$$

FIG. 1. The L = 0 phase shifts for potential (III.1). $V_0 = -51.5$ MeV, $\mu = 0.39$ F⁻², w = m = 0.5. (a) One-Gaussian triton trial wave function for approximations I-III with $F_U = -6.89$ MeV. (b) Two-Gaussian triton trial wave function for approximations I-III with $E_U = -9.07$ MeV. The dashed lines are approximations I and III with $E_U = -9.79$ MeV. (c) Three-Gaussian triton trial wave function for approximations I-III with $E_U = 9.79$ MeV. The dashed lines are approximations I and III with $E_U = -9.79$ MeV.

(IV.1)

and then substituted the approximate wave function Φ_T for φ_T . Because the wave functions Φ_T are determined from the variational principle

$$E_{U} \leq \int d\tau_{T} \Phi_{T} H_{T} \Phi_{T} , \qquad (IV.2)$$

the errors in Φ_T are minimized for the specific operator H_T .

On the other hand, approximation III is derived by using the property

$$T_{23-1}\varphi_T(123) = (-T_{23} - V_{12} - V_{13} - V_{23} + E_T)\varphi_T(123)$$
(IV.3)

before Φ_T is substituted for φ_T . But the errors in



FIG. 2. The L = 1 phase shifts for potential (III.I). V_0 = -51.5 MeV, $\mu = 0.39$ F⁻², w = m = 0.5. (a) One-Gaussian triton trial wave function for approximations I–III with $E_U = -6.89$ MeV. (b) Two-Gaussian triton trial wave function for approximations I–III with $E_U = -9.07$ MeV. The dashed lines are approximations I and III with E_U = -9.79 MeV. (c) Three-Gaussian triton trial wave function for approximations I–III with $E_U = -9.16$ MeV. The dashed lines are approximations I and III with $E_U = -9.79$ MeV.

 Φ_T are minimized for the total triton Hamiltonian H_T , not for the kinetic and potential energy operators separately. This means that the kinetic or potential energy operators acting on a variationally determined wave function are not guaranteed to give as small an error as the Hamiltonian acting on that wave function. This would explain the greater sensitivity of approximation III to the trial wave function.

The dashed lines in Figs. 1 and 2 represent the phase shifts calculated using approximations I and III with a triton binding energy of -9.79 MeV, a value which is close to the exact value for our potential.¹⁰ These phase shifts appear to have smaller uncertainty than those calculated using approximations I and III with the variational binding energy. The size of the improvement indicates that the use of the variational binding energy introduces an error of the same magnitude as the error which results from the approximation of the triton wave function. Approximation II does not depend upon the triton binding energy and thus, is not sensitive to any uncertainty in its determination. For this reason approximation II seems to be a more useful equation to describe neutrontriton scattering than either approximation I or III.

V. CONCLUSION

We have shown that the error introduced by using simple variational wave functions to approximate the bound state of the composite particles in nuclear-scattering calculations can be important. Since this error depends in a nonlinear manner on the overlap of the approximate and exact boundstate wave functions, it is difficult to evaluate directly. Therefore, starting with a many-body Hamiltonian for the nucleon-nucleus system, we derived three different nonlocal single-particle effective potentials which are equivalent when the exact wave function and binding energy of the composite particle are used. The error which results from the use of the approximate wave functions and binding energies was shown to be the same order for each of the effective potentials, and consequently the magnitude of this error could be inferred from the differences in the phase shifts calculated with the various effective potentials. The effective potential first given in this investigation (approximation II) does not depend upon the binding energy of the composite particle, and so is not affected by errors in its determination, as are the two effective potentials used in previous calculations. For this reason it seems the best of the three for use when the error in the binding energy is not known. More investigation is necessary before the magnitude of the error associated

with each approximation can be determined directly, rather than be inferred.

Numerical calculations were done for the particular case of neutron-triton scattering by the RGSM. For a spin-independent potential rigorous lower bounds were set on the overlap of the approximate triton wave functions with the exact triton function. It was found that the differences between the phase shifts calculated with the three different approximations decrease when trial wave functions with better lower bounds to the overlap are used. This confirmed our earlier contention.

Two features of the curves were pointed out and discussed. The differences between the phase shifts calculated with the three approximate effective potentials decreased somewhat more slowly for the P waves than for the S waves. This was attributed to the influence of the tail of the boundstate wave function, which is known to be improved slowly by a variational calculation. It was also noted that approximation III is evidently more sensitive to the variational wave function than is approximation I or II. In approximation III the assumption was made that the kinetic or potential energy operators acting on a variational wave function have an error which is everywhere equal to the error which results from the Hamiltonian acting on the wave function. It was pointed out that this is not necessarily true, and this was offered as an explanation for the greater sensitivity of approximation III to the properties of the variational wave function.

A phase-shift analysis¹⁷ of experimental data shows that neutron-triton scattering is spin-dependent, which may be understood on the basis of a central, but spin-dependent two-nucleon potential. Such a two-nucleon potential introduces a component of mixed spin-space symmetry, known as the S' state,¹⁸ into the triton ground-state wave function. This means that a study of neutron-triton scattering similar to ours, but with a spindependent potential, requires the construction of triton wave functions containing both components determined to an accuracy comparable with that given here. Phase-shift calculations using a spindependent two-nucleon potential and the triton trial wave functions given here indicate that the effect of neglecting the S' state can be significant.¹⁹ If spin-dependent potentials and the S' state of the triton were used, the uncertainty in the phase shifts should be similar to that for the spin-independent case. Since the uncertainties in the phase shifts calculated with a one-Gaussian trial wave function, as indicated in Figs. 1 and 2, are comparable with the error in the determination of the experimental phase shifts of Ref. 17, we conclude that the one-Gaussian trial wave functions are not

sufficiently accurate to allow a comparison between the experimental and theoretical results.

Many calculations of the scattering of nucleons by very light nuclei, other than neutron-triton scattering, have been done using the RGSM.² In all of those calculations one-Gaussian wave functions are used to approximate the target wave function. The effect on the results of those calculations of using a poor approximate target wave function should be similar to that of the neutrontriton case. Many recently published calculations of the scattering between very light nuclei have been done using the cluster model of nuclear reactions,²⁰ where the wave functions of both nuclei are approximated by one-Gaussian wave functions. For these calculations it is probable that the resulting uncertainty in the scattering phase shifts will be even larger than for nucleon-nucleus scattering.

APPENDIX

Here we discuss Eq. (III.23) in more detail, including its expansion into an equation for the partial waves of neutron-triton scattering. For convenience of notation we define

 $\vec{r} \equiv \vec{r}_{123-4}$

 $\vec{\mathbf{r}}' \equiv \vec{\mathbf{r}}_{234-1}.$

*

and

Then, for the quantities $U(\vec{r}_{123-4})$ and $K(\vec{r}_{123-4}, \vec{r}_{234-1})$ of Eq. (III.23) we have

$$U(\mathbf{\dot{r}}_{123-4}) \equiv U(\mathbf{\dot{r}}) = S_{U}V(\mathbf{\dot{r}}),$$

and

$$\begin{split} K(\vec{\mathbf{r}}_{123-4}, \vec{\mathbf{r}}_{234-1}) &\equiv K(\vec{\mathbf{r}}, \vec{\mathbf{r}}') \\ &= S_Q Q(\vec{\mathbf{r}}, \vec{\mathbf{r}}') + S_Q S(\vec{\mathbf{r}}, \vec{\mathbf{r}}') + S_T T(\vec{\mathbf{r}}, \vec{\mathbf{r}}') \\ &+ S_R R(\vec{\mathbf{r}}, \vec{\mathbf{r}}') + M(\vec{\mathbf{r}}, \vec{\mathbf{r}}') + P(\vec{\mathbf{r}}, \vec{\mathbf{r}}') \;. \end{split}$$

$$(A.2)$$

The factors S_U , S_Q , S_T , and S_R depend upon the total spin of the neutron-triton system; S_Q and S_R are different for the three approximations as well. They are listed in Table III. The quantities $U(\mathbf{\dot{r}}), Q(\mathbf{\dot{r}}, \mathbf{\dot{r}}'), T(\mathbf{\dot{r}}, \mathbf{\dot{r}}'), S(\mathbf{\dot{r}}, \mathbf{\ddot{r}}'), R(\mathbf{\ddot{r}}, \mathbf{\ddot{r}}'), N(\mathbf{\ddot{r}}, \mathbf{\ddot{r}}'),$

TABLE III. The spin factors of Eq. (A.2).

	Approximation	I Approximation II	Approximation III
s _v	$\frac{3}{2}(3w-m)$	$\frac{3}{2}(3w-m)$	$\frac{3}{2}(3w-m)$
SQ	3(-w -m)	$\frac{3}{2}(-w -m)$	$\frac{3}{8}(w+m)$
S_T	$\frac{3}{2}(-w+3m)$	$\frac{3}{2}(-w+3m)$	$\frac{3}{2}(-w+3m)$
S _R	$\frac{3}{2}(-w -m)$	0	$\frac{15}{8}(w+m)$

3

and $P(\mathbf{\dot{r}}, \mathbf{\dot{r}}')$ do not depend upon the total spin; all but $N(\mathbf{\dot{r}}, \mathbf{\ddot{r}}')$ and $P(\mathbf{\ddot{r}}, \mathbf{\ddot{r}}')$ are the same for each approximation.

For approximations I-III,

$$\begin{split} V(\vec{\mathbf{r}}) &= \left(\frac{9}{8}\right)^3 \frac{m}{\hbar^2} \int \Phi(123) V(\vec{\mathbf{r}}_{14}) \Phi(123) d\vec{\mathbf{r}}_{23} d\vec{\mathbf{r}}', \\ (A.3) \\ Q(\vec{\mathbf{r}}, \vec{\mathbf{r}}') &= \left(\frac{9}{8}\right)^3 \frac{m}{\hbar^2} \int \Phi(123) V(\vec{\mathbf{r}}_{12}) \Phi(234) d\vec{\mathbf{r}}_{23}, \\ (A.4) \end{split}$$

$$S(\mathbf{\vec{r}},\mathbf{\vec{r}}') = \left(\frac{9}{8}\right)^3 \frac{m}{\hbar^2} \int \Phi(123) V(\mathbf{\vec{r}}_{24}) \Phi(234) d\mathbf{\vec{r}}_{23},$$
(A.5)

$$T(\mathbf{\ddot{r}},\mathbf{\ddot{r}}') = \left(\frac{9}{8}\right)^3 \frac{m}{\hbar^2} \int \Phi(123) V(\mathbf{\ddot{r}}_{14}) \Phi(234) d\mathbf{\vec{r}}_{23},$$
(A.6)

$$R(\vec{\mathbf{r}},\vec{\mathbf{r}}') = \left(\frac{9}{8}\right)^3 \frac{m}{\hbar^2} \int \Phi(123) V(\vec{\mathbf{r}}_{23}) \Phi(234) d\vec{\mathbf{r}}_{23} .$$
(A.7)

For the approximation I

$$M(\mathbf{\ddot{r}},\mathbf{\ddot{r}}') = \left(\frac{9}{8}\right)^3 \frac{3}{2} \frac{m}{\hbar^2} (E_n + E_T) \int \Phi(123) \Phi(234) d\mathbf{\vec{r}}_{23}, \tag{A.8}$$

$$P(\vec{\mathbf{r}},\vec{\mathbf{r}}') = \left(\frac{9}{8}\right)^{3} \int \Phi(123)\Phi(234) \left\{\frac{27}{32} \frac{\vec{\nabla}_{23-1}\Phi(123) \cdot \vec{\nabla}_{23-4}\Phi(234)}{\Phi(123)\Phi(234)} + \left(\frac{9}{8}\right)^{2} \left[\frac{\nabla^{2}_{23-1}\Phi(123)}{\Phi(123)} + \frac{\nabla^{2}_{23-4}\Phi(234)}{\Phi(234)}\right] + \frac{3}{2} \frac{\nabla^{2}_{23}\Phi(234)}{\Phi(234)} \left\{d\vec{\mathbf{r}}_{23}, (A.9)\right\}$$

for approximation II

$$M(\vec{\mathbf{r}}, \vec{\mathbf{r}}') = \left(\frac{9}{8}\right)^3 \frac{3}{2} \frac{m}{\hbar^2} E_n \int \Phi(123) \Phi(234) d\vec{\mathbf{r}}_{23}, \qquad (A.10)$$

$$P(\vec{\mathbf{r}}, \vec{\mathbf{r}}') = \left(\frac{9}{8}\right)^3 \left(\Phi(123) \Phi(234) \left[\frac{27}{23} \cdot \vec{\nabla}_{23-1} \Phi(123) \cdot \cdot \vec{\nabla}_{23-4} \Phi(234) + \frac{45}{23} \left(\frac{\nabla^2_{23-1} \Phi(123)}{23} + \frac{\nabla^2_{23-4} \Phi(234)}{23} \right) \left[\frac{27}{23} \cdot \vec{\nabla}_{23-1} \Phi(123) \cdot \cdot \vec{\nabla}_{23-4} \Phi(234) + \frac{45}{23} \left(\frac{\nabla^2_{23-1} \Phi(123)}{23} + \frac{\nabla^2_{23-4} \Phi(234)}{23} \right) \left[\frac{27}{23} \cdot \vec{\nabla}_{23-1} \Phi(123) \cdot \cdot \vec{\nabla}_{23-4} \Phi(234) + \frac{45}{23} \left(\frac{\nabla^2_{23-1} \Phi(123)}{23} + \frac{\nabla^2_{23-4} \Phi(234)}{23} \right) \left[\frac{27}{23} \cdot \vec{\nabla}_{23-1} \Phi(123) \cdot \cdot \vec{\nabla}_{23-4} \Phi(234) + \frac{45}{23} \left(\frac{\nabla^2_{23-1} \Phi(123)}{23} + \frac{\nabla^2_{23-4} \Phi(234)}{23} \right) \left[\frac{27}{23} \cdot \vec{\nabla}_{23-4} \Phi(234) + \frac{45}{23} \left(\frac{\nabla^2_{23-1} \Phi(123)}{23} + \frac{\nabla^2_{23-4} \Phi(234)}{23} \right) \left[\frac{27}{23} \cdot \vec{\nabla}_{23-4} \Phi(234) + \frac{45}{23} \left(\frac{\nabla^2_{23-1} \Phi(123)}{23} + \frac{\nabla^2_{23-4} \Phi(234)}{23} \right) \left[\frac{27}{23} \cdot \vec{\nabla}_{23-4} \Phi(234) + \frac{45}{23} \left(\frac{\nabla^2_{23-1} \Phi(123)}{23} + \frac{\nabla^2_{23-4} \Phi(234)}{23} \right) \left[\frac{27}{23} + \frac{\nabla^2_{23} \Phi(234)}{23} + \frac{27}{23} + \frac{\nabla^2_{23} \Phi(234)}{23} \right]$$

$$P(\vec{\mathbf{r}},\vec{\mathbf{r}}') = \left(\frac{9}{8}\right)^{6} \int \Phi(123)\Phi(234) \left[\frac{27}{32} \frac{\nabla_{23-1}\Phi(123) \cdot \nabla_{23-4}\Phi(234)}{\Phi(123)\Phi(234)} + \frac{45}{64} \right] \frac{\nabla_{23-1}^{2}\Phi(123)}{\Phi(123)} + \frac{\nabla_{23-4}^{2}\Phi(234)}{\Phi(234)} \left\{ \int d\vec{\mathbf{r}}_{23} \right\},$$
(A.11)

while for approximation III

$$M(\vec{\mathbf{r}},\vec{\mathbf{r}}') = \frac{3}{2} \left(E_n - \frac{5}{4} E_T\right) \left(\frac{9}{8}\right)^3 \frac{m}{\hbar^2} \int \Phi(123) \Phi(123) d\vec{\mathbf{r}}_{23},$$

$$P(\vec{\mathbf{r}},\vec{\mathbf{r}}') = \frac{3}{8} \left(\frac{9}{8}\right)^3 \int dr_{23} \Phi(123) \Phi(234) \left[\frac{9}{4} \frac{\vec{\nabla}_{23-1} \Phi(123) \cdot \vec{\nabla}_{23-4} \Phi(234)}{\Phi(123) \Phi(234)} - 5 \frac{\nabla^2_{23} \Phi(123)}{\Phi(123)}\right].$$
(A.12)

As mentioned in Sec. III, Eq. (III.23) was resolved into partial waves. The kernel $K(\mathbf{\vec{r}}, \mathbf{\vec{r}}')$ was expanded in terms of Θ , the angle between $\mathbf{\vec{r}}$ and $\mathbf{\vec{r}}'$, as

$$K(\mathbf{\vec{r}},\mathbf{\vec{r}}') = \sum_{l} \frac{2l+1}{4\pi r r'} P_{l}(\cos\Theta)k_{l}(r,r'). \qquad (A.13)$$

If this expansion and the expansion of $F_s(\mathbf{\dot{r}})$ in θ , the angle between $\mathbf{\ddot{r}}$ and an arbitrary fixed coordinate system,

$$F_{s}(\vec{\mathbf{r}}) = \frac{1}{\gamma} \sum_{l} F_{l(r)} P_{l}(\cos\theta)$$
(A.14)

are substituted in Eq. (III.23), there results the

integrodifferential equation for $F_{I}(r)$,

$$\left[\frac{d^{2}}{dr^{2}} + k^{2} - \frac{l(l+1)}{r^{2}}\right]F_{l}(r)$$

= $U(r)F_{l}(r) + \int_{0}^{\infty} k_{l}(r, r')F_{l}(r')dr',$
(A.15)

where

$$k^2 = \frac{3}{2} (m/\hbar^2) E_n$$
.

The quantities U(r) and especially $k_l(r, r')$ are quite lengthy and complex, and therefore are not given here. They may be found in detail in Ref. 19.

ACKNOWLEDGMENTS

We thank Professor Fritz Coester for suggesting this problem, for his many penetrating discussions, and for a critical reading of the manuscript. We also thank Professor Leonard Schlessinger for his assistance in performing the variational calculations, and for providing the programs for this portion of the work; and Professor William Stwalley for information on variational bounds. \ast Research supported in part by the National Science Foundation.

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PHYSICAL REVIEW C

VOLUME 3, NUMBER 6

JUNE 1971

Excitation Functions of ⁷Be and ¹¹C Produced in Nitrogen by Low-Energy Protons

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(Received 8 March 1971)

The cross sections for the production of ¹¹C and ⁷Be by protons from a ¹⁴N target has been measured at energies from 5–24 MeV for ¹¹C and 13–42 MeV for ⁷Be. A sharp rise above the thresholds for the ¹⁴N(p, α) and ¹⁴N(p, 2α) reactions was observed, with maxima, respectively, around 200 and 45 mb.

INTRODUCTION

The measurement of the cross sections for the formation of ⁷Be and ¹¹C in nitrogen is part of a larger program undertaken at Orsay in order to establish the excitation functions of Li, Be, and B in the bombardment of ¹²C, ¹⁴N, and ¹⁶O by protons and α particles. In addition to their interest to the nuclear physicist, these excitation functions are essential to the astrophysicist for the study of many problems such as the nucleosynthesis of the *L* elements¹ (Li, Be, B), determination of their stellar abundances,² and the propagation of cosmic rays.³ Also, ⁷Be is used as a monitor for the

measurement of the absolute cross sections of the stable isotopes of the light elements when a mass spectrometric method is used. In many geophysical investigations,⁴ ⁷Be is an interesting radioisotope, as it is formed continually by the interaction of the cosmic particles with the atmosphere, which is essentially composed of nitrogen.

The cross sections for production of ¹¹C and ⁷Be have been known for a long time in ¹²C and ¹⁶O over a great range of energies, while in nitrogen very few measurements have been made, especially in the low-energy range: ¹¹C has been measured only between 5 and 6 MeV, ⁵ at 13 MeV, ⁶ and 50 MeV, ⁷ with a rather large uncertainty. In view