Convergence features in the pseudostate theory of the $d+\alpha$ system

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(Received 13 June 1988)

Convergence properties of the pseudostate method in the $d+\alpha$ system are investigated with respect to the number of deuteron Gaussian basis functions and the number of pseudo-inelastic configurations. Results indicate that the deuteron specific distortion effect can be well described by using about 10 to 15 Gaussian basis functions to generate deuteron wave functions in the ground and pseudo-excited states. Also, it is found that, for the ground-state energy of ^{6}Li and for $d+\alpha$ scattering in the very low energy region, only deuteron pseudo-excited states with excitation energies less than about 60 MeV need to be included. In addition, the investigation shows that the calculated total reaction cross sections are rather severely underestimated, indicating that even more cluster configurations must be introduced into the resonating-group formulation in order to obtain a satisfactory explanation of all the important features of the six-nucleon system.

I. INTRODUCTION

For a two-cluster $A+B$ system, the pseudostate method[1-3] can be used to study the specific distortion effect[4] and the influence on the elastic channel of cluster breakup processes. In this method, pseudo-excited states of the clusters are systematically introduced, and these states are utilized to construct various pseudo-inelastic configurations. The resultant resonanting-group formulation, which consists of both elastic and pseudo-inelastic channels, is then solved to obtain the associated relative-motion functions or linear variational amplitudes. As has been mentioned previously,[3] the main advantage of this method lies in its simplicity of formulation, because the kernel functions representing the coupling among various cluster configurations can be rather easily derived.

The application of this method has already been made in a number of light nuclear systems,[3] and interesting and useful results about the essential characteristics of the examined systems have been achieved. In this investigation, we shall try to build up a more solid foundation for this method and consider the important problem concerning the convergence features of a pseudostate calculation. This is quite obviously an important problem, because practical considerations will always limit the number of pseudo-inelastic configurations which can be adopted. In a preliminary study,[3] we briefly investigated this problem in the $S=\frac{3}{2}$ state of the $d+{}^3$He system. Here we shall continue this type of investigation by considering the $d+\alpha$ system with a large number of deuteron pseudostates and examining the convergence behavior of not only the scattering phase shifts and reflection coefficients, but also the differential scattering and total reaction cross sections in the energy region up to around 30 MeV/nucleon. We choose this particular system for a detailed examination simply because only one of the clusters involved, namely, the deuteron cluster, has a high compressibility with respect to radial distortion.

A brief description of the pseudostate method to take into account the deuteron specific-distortion effect in the $d+\alpha$ system is given in Sec. II. In Sec. III, we study the convergence features regarding the number m of Gaussian basis functions which are used to generate the deuteron wave functions in the ground and pseudo-excited states. For this study, we have performed a number of calculations with m up to 15, but will mainly discuss the results obtained with $m=6$, 10, and 15. With m set as 15, we next study, in Sec. IV, the convergence features with respect to the number of pseudo-inelastic configurations. The aim here is to determine the deuteron excitation-energy region which needs to be covered in order to achieve a chosen degree of accuracy for the $d+\alpha$ bound-state and scattering properties. Finally, in Sec. V, we discuss the results obtained in this investigation and make some concluding remarks.

II. BRIEF DESCRIPTION OF THE PSEUDOSTATE METHOD

The spatial wave functions of the deuteron in its ground and pseudo-excited states are obtained by diagonalizing the deuteron Hamiltonian in a space spanned by m Gaussian basis functions of the form

$$\chi_i=\exp\left[-\tfrac{1}{2}\lambda_i\sum_{j=1}^{2}(\mathbf{r}_j-\mathbf{R}_d)^2\right],\quad i=1-m \tag{1}$$

where $\mathbf{R}_d$ denotes the center of mass coordinate of the deuteron cluster. The nonlinear variational parameters λ_i should, in principle, be determined by minimizing the ground-state energy eigenvalue in the chosen model space. When m is large, however, one can simplify the procedure by simply choosing a set of convenient λ_i values which cover a wide enough width parameter range. This is, in fact, what we have done for $m=10$, 12,

TABLE I. Properties of deuteron ground and pseudo-excited states.

m	λ_i (fm^{-2})	E_i (MeV)	$\tilde{R}_d$ (fm)
10	0.028, 0.084, 0.24, 0.60, 1.4, 2.8, 3.8, 4.8, 7.2, 10.8	−2.1676, 1.2319, 6.819, 24.03, 67.68, 156.5, 311.5, 564.2, 974.8, 1716	1.965
12	0.014, 0.04, 0.106, 0.256, 0.56, 1.04, 1.84, 3.08, 4.80, 7.0, 10.4, 15.6	−2.1676, 0.5172, 2.80, 9.53, 26.6, 63.7, 134.0, 257.0, 461, 798, 1360, 2410	1.966
15	0.004, 0.02, 0.04, 0.08, 0.144, 0.252, 0.44, 0.76, 1.32, 2.30, 4.0, 6.8, 11.2, 18.0, 30.0	−2.1676, 0.1396, 0.8977, 3.00, 7.51, 16.37, 33.06, 63.70, 118.5, 214.2, 380.4, 670.5, 1183, 2109, 3931	1.966

and 15. In Table I, we list in these three cases the chosen λ_i values, the corresponding energy eigenvalues E_i of the deuteron ground and pseudo-excited states, and the rms radius $\tilde{R}_d$ of the deuteron in its ground state. To obtain these results, we have used the nucleon-nucleon potential given by Eqs. (12)–(17) of Ref. 5 (i.e., the MN or Minnesota potential) and a value for $\hbar^2/2M_N = 20.804$ MeV fm^2, with M_N being the nucleon mass. From Table I, one notes that the ground-state properties are almost entirely the same in all three cases, indicating that the deuteron model space is already quite large with $m = 10$. The main difference occurs in the excitation energies of the pseudo-excited states; when m is increased from 10 to 15, the excitation energy of the first pseudo-excited state decreases from 3.3995 to 2.3072 MeV.

With the deuteron ground- and pseudo-excited-state wave functions ϕ_i ($i = 1-m$) determined as described above, one can then properly consider the deuteron specific-distortion effect by constructing a trial function for the $d+\alpha$ system in the following multiconfiguration resonating-group form:

$$\psi = \sum_{i=1}^{M} \mathcal{A} \left\{ \phi_\alpha \phi_i \left[\frac{1}{R} f_{JL}^{i}(R) \mathcal{Y}_{JLS}^{M} \right] Z(\mathbf{R}_{\text{c.m.}}) \right\}, \quad M \leq m \tag{2}$$

where $\mathcal{A}$ is an antisymmetrization operator, $\mathcal{Y}_{JLS}^{M}$ is a spin-isospin angle function appropriate for $T=0$ and $S=1$, and $Z(\mathbf{R}_{\text{c.m.}})$ is any normalizable function describing the total c.m. motion. The function ϕ_α describes the spatial structure of the α cluster in its ground state; it is assumed to be a linear superposition of two Gaussian functions with width parameters equal to 0.306 and 0.708 fm^{-2} (see Ref. 6). The linear variational amplitudes $f_{JL}^{i}(R)$ are determined from the projection equation

$$\langle \delta\psi \mid H - E_T \mid \psi \rangle = 0 , \tag{3}$$

where E_T denotes the total energy of the six-nucleon system and H is the Hamiltonian operator given by

$$H = -\frac{\hbar^2}{2M_N} \sum_{i=1}^{6} \nabla_i^2 + \sum_{i>j=1}^{6} V_{ij} - T_{\text{c.m.}} , \tag{4}$$

with $T_{\text{c.m.}}$ being the kinetic-energy operator of the total c.m. motion. The nucleon-nucleon potential V_{ij} used is the MN potential already mentioned; it contains two adjustable parameters, an exchange-mixture parameter u in the central part and a depth parameter c_s in the spin-orbit part.

The number M of cluster configurations, contained in ψ of Eq. (2), can take on values from 1 to m. In this investigation, we shall compare the results obtained from calculations with progressively larger values of M, which are performed by successively adding pseudo-inelastic configurations with increasing threshold energies. The purpose of this study is to see whether or not pseudo-excited states with large excitation energies have any significant effects on the properties of the $d+\alpha$ system in the low-energy region. Thus, a particular resonating-group calculation will be specified not only by the value of m but also by the value of M. In the following discussion, such a calculation will be referred to as being performed with an $mG_d - MC$ model or, more simply, an mG_d model if M is equal to m.

With the usual resonating-group procedure, one obtains from Eq. (3) the coupled integrodifferential equations satisfied by the variational amplitudes $f_{JL}^{i}(R)$. These coupled equations are solved by employing a microscopic multichannel R-matrix method.[6,7] Using the S-matrix elements obtained, one then finds the phase shifts and reflection coefficients in the elastic channel and, subsequently, the $d+\alpha$ differential scattering and total reaction cross sections.

III. CONVERGENCE FEATURES WITH RESPECT TO THE NUMBER OF DEUTERON GAUSSIAN BASIS FUNCTIONS

To examine the convergence features of the $d+\alpha$ pseudostate study with respect to the number m of deuteron Gaussian basis functions, we perform a number of calculations with $M = m = 3$, 4, 5, 6, 10, 12, 13, and 15. In a previous publication,[6] we already reported some selected results obtained with smaller values of $m \leq 10$. Here a more thorough discussion will be given, based on these

previous results and our new results obtained with larger m values equal to 12, 13, and 15. For clarity in discussion and interpretation, we shall simplify the calculation by omitting, except for cross-section results, the spin-orbit part of the nucleon-nucleon potential by setting $c_s=0$.

In Fig. 1, the values of the exchange-mixture parameter u are shown in the various mG_d models. To obtain these values, we have used the criterion that the cluster relative energy $\tilde{E}$ in the ^{6}Li ground state be exactly equal to the experimentally determined value of -1.474 MeV. As is seen from this figure, the values of u for $m=12$, 13, and 15 are very nearly the same, indicating that the u value of 0.9815 for $m=15$ can be considered as the convergent or saturated value and that the $15G_d$ model is certainly adequate to describe the effect of deuteron specific distortion in the ground state of the $d+\alpha$ system.

To discuss more quantitatively, we note that when u is increased by 0.01, the value of $\tilde{E}$ decreases by about 0.11 MeV.[8] Take the $6G_d$ model as an example; this means that if we had used $u=0.9815$ in this model, $\tilde{E}$ would be equal to about -1.377 MeV, which is only 0.097 MeV higher than the correct value. Thus, as far as the ^{6}Li ground state is concerned, even the $6G_d$ model seems to be reasonably adequate and there is no particular reason to go beyond $m=15$ since calculations with large values of m do have rather severe computational requirements.

Phase shifts δ_L and reflection coefficients η_L in the elastic channel, defined through the S-matrix element $S_L=\eta_L \exp(2i\delta_L)$, are shown in Figs. 2–4 for $L=0$–3 in the $6G_d$, $10G_d$, and $15G_d$ models, with u values of Fig. 1.

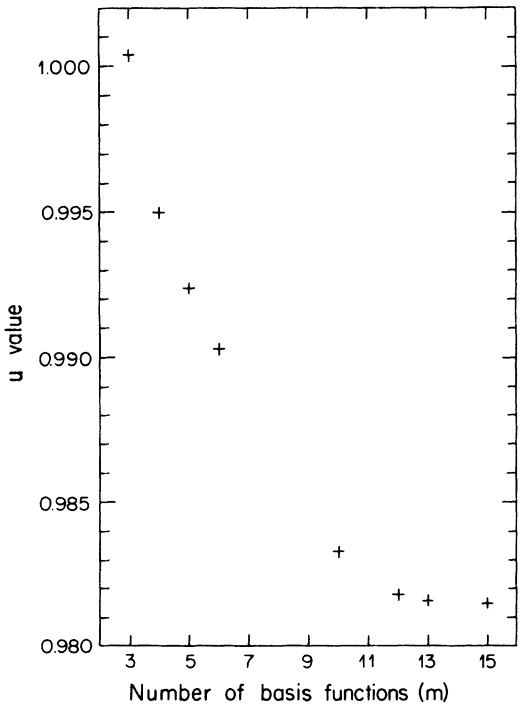

FIG. 1. The value of the exchange-mixture parameter u which is needed in each mG_d model to reproduce the experimentally determined cluster relative energy in the ground state of ^{6}Li.

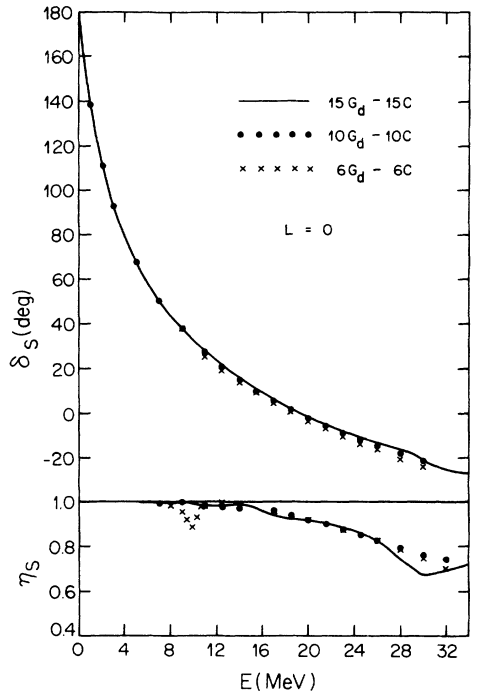

FIG. 2. Phase shifts δ_S and reflection coefficients η_S in the $L=0$ state obtained with the $6G_d$, $10G_d$, and $15G_d$ models.

Here one notes the following features.

(i) Especially for the phase shifts, the average behaviors in these three models are very similar.

(ii) In the $6G_d$ case, the influence of distortion resonances, which arise from the use of a limited number of pseudo-inelastic configurations, does show up more distinctly (see, e.g., the η_D points in the energy region from 20 to 32 MeV).

(iii) As the value of m becomes larger, the phase-shift and reflection-coefficient curves do become smoother. At energies up to about 25 MeV/nucleon (i.e., about 33 MeV in the c.m. system), the $15G_d$ phase-shift curve shows only a slight wavy behavior at around 30 MeV. This indicates that the choice of $m=15$ is also sufficient to ex-

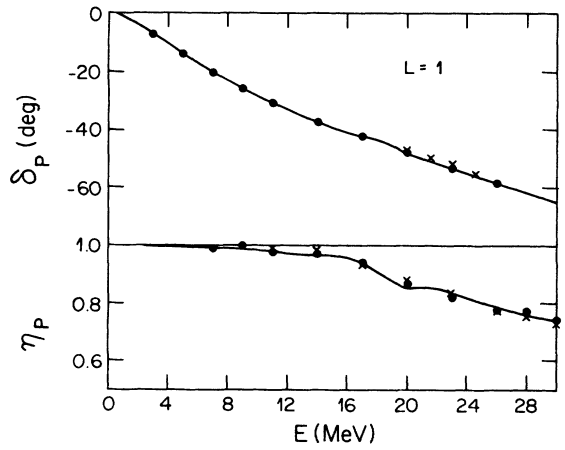

FIG. 3. Same as Fig. 2, except that $L=1$.

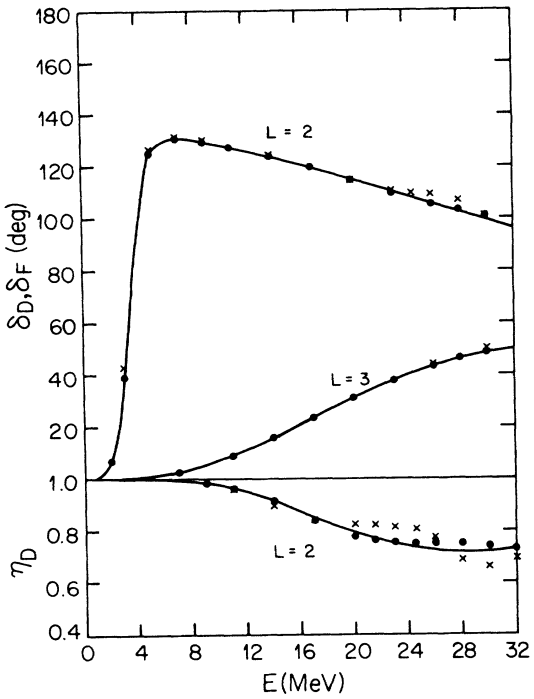

FIG. 4. Same as Fig. 2, except that $L=2$ and 3.

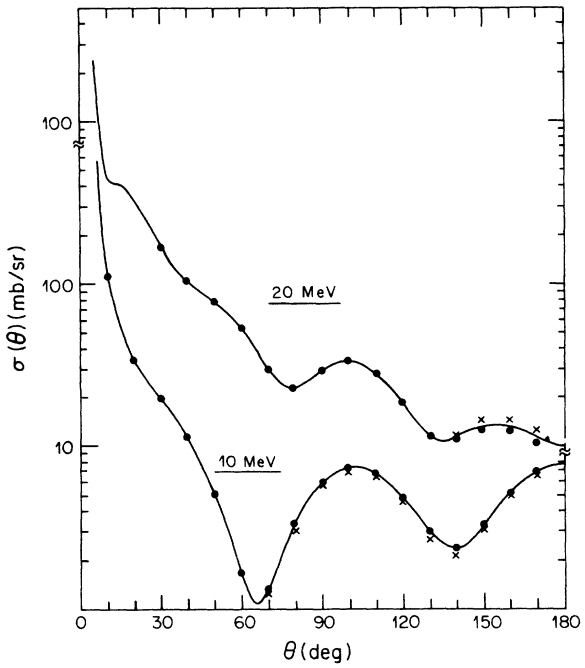

FIG. 5. Differential scattering cross sections at 10 and 20 MeV in the $6G_d$, $10G_d$, and $15G_d$ models.

plain the scattering properties in this energy region.

Differential scattering cross sections $\sigma(\theta)$ at 10 and 20 MeV are shown in the $6G_d$ (crosses), $10G_d$ (solid circles), and $15G_d$ (solid curve) cases in Fig. 5. To obtain these cross-section results, we have used the u values given in Fig. 1 and a common value of 0.92 for c_s in all three models. From this figure, one notes that, except for small differences at large backward angles, the results from all these models are nearly identical. This is so even at 10 MeV where the $6G_d$, $L=0$ reflection-coefficient result exhibits a notable minimum (see Fig. 2). Evidently, the value of $\eta_S \cong 0.9$ at this minimum represents sufficiently weak coupling to the distortion resonance such that no significant effects show up in the elastic-scattering cross-section curve at this energy where a number of partial waves contribute.

The $d+\alpha$ total reaction cross sections σ_R as a function of the scattering energy E are shown in Fig. 6 for the $6G_d$ (dotted curve), $10G_d$ (dashed curve), and $15G_d$ (solid curve) models. Here it is seen that the $10G_d$ and $15G_d$ results are rather similar. As expected, the curve becomes smoother as the value of m becomes larger. In the $15G_d$ case, the curve looks still somewhat wavy; however, for a reaction cross-section curve, the degree of waviness shown here is quite tolerable.

Calculated total reaction cross sections in the energy range from 20 to 40 MeV are around 90 mb. These values are much smaller than the values of about 400 mb obtained from a single-configuration resonating-group calculation which includes a phenomenological imaginary potential adjusted to yield a best fit with experimental differential cross-section results.[9] This indicates that our present $15G_d$ pseudostate study cannot explain all the important features of the six-nucleon system, although it does yield an accurate account of the effect of deuteron specific distortion. For a more complete description, more cluster configurations must be incorporated into the resonating-group formulation. Based on energetical considerations, our opinion is that, in addition to the many $d+\alpha$ cluster configurations employed here, it would be necessary to at least further include the $p+{}^5$He and $n+{}^5$Li structures together with their associated pseudo-inelastic configurations. Quite clearly, such an extensive formulation would result in a formidable calculation; however, from a microscopic viewpoint, this is unavoidable if one desires to explain all the essential properties of this complicated six-nucleon system even at relatively low energies.

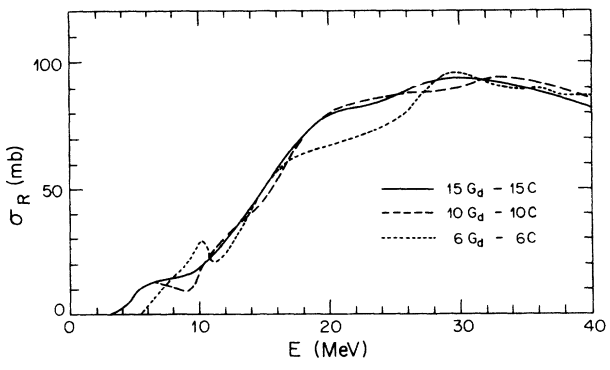

FIG. 6. Total reaction cross sections in the $6G_d$, $10G_d$, and $15G_d$ models.

IV. CONVERGENCE FEATURES WITH RESPECT TO THE NUMBER OF PSEUDO-INELASTIC CONFIGURATIONS

With $m=15$ and $u=0.9815$, we now study the question as to the number M of cluster configurations with progressively higher energy thresholds which one must use in order to achieve a chosen degree of accuracy in the calculated properties of the $d+\alpha$ system. This is certainly useful information to have, since a calculation with a smaller value of M is unquestionably desirable from a computational viewpoint.

In Fig. 7, we show the dependence of $\tilde{E}$, the cluster relative energy in the ground state of ^{6}Li, on the number M. Here one finds that $M=12$ nearly saturates the eventual value of -1.474 MeV obtained with the $15G_d-15C$ calculation. This means that, as far as the ^{6}Li ground state is concerned, the inclusion of deuteron pseudo-excited states with excitation energies higher than about 1 000 MeV (see Table I) has no significance. Based on a rather similar approach, Yahiro and Kamimura[10] have suggested a practical criterion that, in a pseudostate-type calculation, only deuteron pseudostates with excitation energies less than about 40 MeV need to be included. If we had adopted this criterion and stopped the calculation at $M=8$ (i.e., $8C$ calculation), then we would have obtained an $\tilde{E}$ value of -1.393 MeV, which is reasonably close to the $15C$ result of -1.474 MeV.

From Fig. 7, it is also noted that the $\tilde{E}$ values from the $1C$ and $15C$ calculations differ by 1.846 MeV. This shows that the deuteron specific-distortion effect is very important in the ground state of ^{6}Li, which is not unexpected because of the high compressibility of the deuteron cluster.

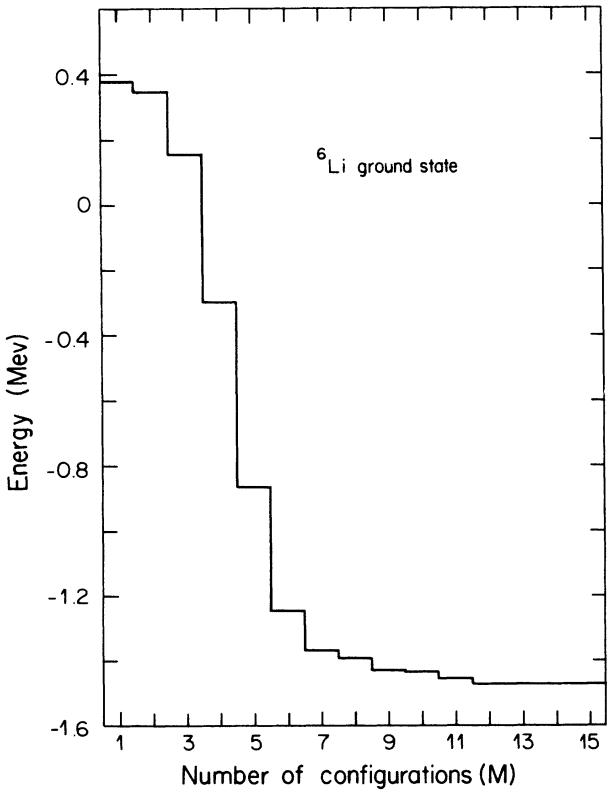

FIG. 7. Dependence of the cluster relative energy in the ground state of ^{6}Li on the number of cluster configurations.

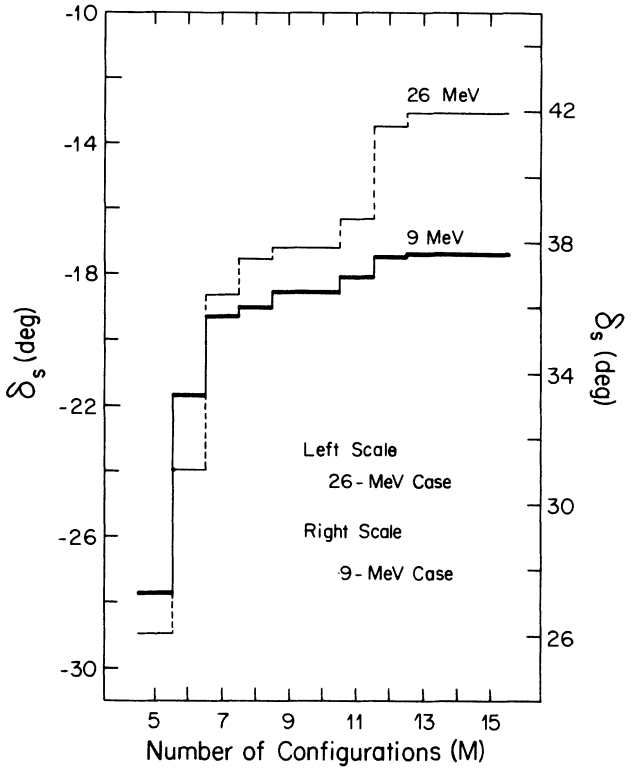

FIG. 8. Dependence of the $L=0$ phase shifts at 9 and 26 MeV on the number of cluster configurations.

The situation is rather similar in the low-energy scattering case. In Fig. 8, we show the $d+\alpha$, $L=0$ phase shift δ_S at c.m. energies of 9 and 26 MeV. From this figure one sees that the value of δ_S changes substantially when more and more deuteron pseudostates are introduced into the calculation. At 9 MeV, for example, the $1C$ and $15C$ values are, respectively, equal to 13.34° and 37.63°, a large difference of 24.29°. Also, there is again saturation near the $12C$ calculation. On the other hand, the Yahiro and Kamimura criterion needs to be somewhat liberalized. With an $8C$ calculation, δ_S at 9 MeV is equal to 36.01°, indicating that, already at such a low energy, there is an appreciable difference of 1.62° from the $15C$ result.

By studying the variation of δ_S with M, we obtain a more precise criterion for the choice of deuteron pseudostates in the $d+\alpha$ system. For an accuracy of about 1° in δ_S, we find that, at very low energies less than 5 MeV, it is only necessary to include deuteron pseudostates with excitation energies up to about 60 MeV ($M=8$). On the other hand, to achieve about the same degree of accuracy at higher energies, one must adopt a few more pseudostates; for example, at 20 MeV, our calculation shows that $M=11$ should be used, for which the excitation energy of the highest deuteron pseudo-excited state is around 400 MeV.

V. CONCLUSION

In this investigation, we study in the $d+\alpha$ system the convergence properties of the pseudostate method with respect to the number of deuteron Gaussian basis functions and the number of pseudo-inelastic configurations. The results indicate that the deuteron specific-distortion effect can be well accounted for by the use of about 10–15 Gaussian basis functions to generate deuteron wave functions in the ground and pseudo-excited states, and calculations with more than 15 basis functions do not appear to be necessary. As for the choice of the number of pseudo-inelastic configurations, it is found that, for the ground state of ^{6}Li and for $d+\alpha$ scattering in the very low-energy region, it is sufficient to include in the calculation only deuteron pseudostates with excitation energies less than about 60 MeV. At higher scattering energies, however, a few more deuteron pseudostates are required in order to achieve the same degree of accuracy for the phase-shift results.

Because of the high compressibility of the deuteron cluster, it is show that, as expected, the specific distortion of the deuteron has a large effect on the properties of the $d+\alpha$ system. In the ground state of ^{6}Li, the introduction of pseudo-inelastic configurations into the calculation improves the cluster separation energy by a large amount equal to about 1.85 MeV.

At this point, it may be useful to mention that the main purpose of adding pseudo-inelastic configurations is to improve the behavior of the six-nucleon system in the strong-interaction region. *A priori,* one of course does not precisely know what important characteristics the added six-nucleon functions must have. In the pseudostate method, one utilizes a large number of pseudo-inelastic structures, hoping that enough configurations have been introduced to achieve convergence in the calculated results. In this sense, the pseudostate method is a brute force method which has, however, the important advantage of simplicity in formulation. The disadvantage is certainly that there is no clear feeling concerning the specific role played by each added function. For example, there does not seem to be any simple explanation why the addition of the 12th configuration causes a rather large change in δ_S at 26 MeV, except to say that this particular configuration must serve to simulate some relatively significant features of the six-nucleon energy eigenfunction in the strong-interaction region.

Also, it should be emphasized that the conclusions reached here about the number of pseudo-inelastic configurations are based on calculations performed with a central nucleon-nucleon potential. If a more realistic potential including a tensor component is adopted, then one will be additionally faced with complicated computational problems associated with couplings between states of different orbital angular momentum. Such couplings might result in some modification of our conclusions and are certainly worth examining in future studies.

In spite of the apparent successes of the present pseudostate calculation in many respects, there is one main defect which should be emphasized. This defect is associated with our finding that the calculated total reaction cross sections are rather severely underestimated. From this one can conclude that, although the present calculation yields an accurate description of the deuteron specific-distortion effect, more cluster configurations are still needed for a satisfactory explanation of all the important features of the six-nucleon system. Based on energetical considerations and previous experience gained from multiconfiguration resonating-group calculations, we are of the opinion that the important cluster configurations to be added are the $p+^5$He and $n+^5$Li structures and, at higher energies, the ^{3}H$+^3$He structure as well. In addition, of course, the many pseudo-inelastic configurations associated with these structures should also be considered in order to obtain a more realistic account of the influence of cluster breakup processes on the $d+\alpha$ elastic channel.

A resonating-group formulation containing all these cluster configurations will result in a very difficult calculation. As a preliminary step, one might wish to first perform a much simpler calculation by merely adding phenomenological imaginary potentials into the present formulation. Quite obviously, this is not a desirable procedure from the microscopic viewpoint. However, based on the experience obtained from previous five-nucleon[11] and seven-nucleon[12] calculations, we believe that it may very likely lead to reasonable results in comparison with experiment and, thereby, provide us with some further useful information concerning the reaction mechanisms in the six-nucleon system.

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