observed line shape for the $Li^6(d,\alpha)He^4$ reaction was folded in to correct the theoretical curve for instrumental resolution. The corrected theoretical line shape was then superimposed on the experimental curve, normalizing to the $Li^7(d,\alpha)He^5$ peak. Since the cross section for a reaction is proportional to the integrated area under the experimental spectrum, the areas under the $Li^7(d,\alpha)He^5$ peak and the $Li^6(d,\alpha)He^4$ peak, corrected for abundance, were calculated. The known value for the cross section of $Li^6(d,\alpha)He^4$ [6] was then used to determine the cross section for the $Li^7(d,\alpha)$ reaction. Figure 3 shows the cross sections determined in our laboratory along with the values of Fessenden and Maxden[10] and Paul and Kohler.[9]

A correction to the deuteron energy was made to account for deuteron energy loss in the thick target. An effective deuteron energy was obtained for each maximum energy by calculating the mean energy using the known excitation function for the $Li^6(d,\alpha)He^4$ as a weighting function and assuming that all deuterons from zero to the maximum energy cause reactions. Assuming that the excitation function for the $Li^7(d,\alpha)He^5$ reaction is similar to that for $Li^6(d,\alpha)He^4$, effective energies were found.

The theoretical cross section for the formation of the compound nucleus Be^{9*}, based on continuum theory, was calculated. This curve was then normalized to the experimental data at 175 keV. In Fig. 3 the experimental points show excellent agreement with the theoretical cross section given by the solid line. Since the experimental points did not fall away from the theoretical curve as energy increased, we conclude no other channels open, up to 300 keV. The data of Paul and Kohler at energies above the region of our experiment show evidence of the well-known resonances at 800 to 1040 keV.

CONCLUSIONS

The differential cross section for the $Li^7(d,\alpha)$ reaction at 90 deg was determined by a relatively simple thick target method, using solid state detectors. The energy dependence of the cross section was found to agree with that for the formation of the compound nucleus, in the energy range 175–300 keV.

ACKNOWLEDGMENTS

The authors gratefully acknowledge helpful discussions with J. A. Lockwood and P. Fessenden.

PHYSICAL REVIEW VOLUME 136, NUMBER 6B 21 DECEMBER 1964

Configuration Mixing Effects in Stripping*

N. AUSTERN
University of Pittsburgh, Pittsburgh, Pennsylvania
(Received 6 August 1964)

The bound "single-particle wave function" into which the stripped particle is inserted is a true single-particle wave function, in the shell-model sense, only if the target nucleus is a closed-shell nucleus. In all other cases the radial shape of this function is altered by configuration mixing effects, and important changes of cross-section magnitudes may ensue. These effects are discussed in the present article, and a detailed comparison is given with the customary phenomenological procedure wherein the configuration mixing effects are estimated in terms of the Q of the reaction.

1. INTRODUCTION

RECENTLY there has been considerable interest in the subject of configuration mixing effects in deuteron stripping, and in other single-nucleon transfer reactions.[1–3] The present article presents some discussion of what these effects are, and of some circumstances under which they may or may not be important.

What is under discussion is the recognition and removal of certain simplifying assumptions which are tacitly made when the usual theory is constructed. Both nuclear structure theory and the distorted-waves stripping theory rely heavily on the use of product wave functions for nuclear bound states. Each theory goes on to improve the wave functions; however, the sorts of improvements which they carry are different. For this reason there is some vagueness when the two theories are used together for practical calculations. Stripping calculations are very sensitive to shapes of radial wave functions; nuclear structure calculations usually ignore radial shapes, and concentrate instead upon building linear combinations of angular momentum states. It is important for the reaction analysis that determination of a best linear combination for a bound-state wave function also implies determination of a best radial shape. It is this relationship which is generally overlooked, or which is treated very crudely.

A sufficient illustration of the dynamics we wish to

* Supported in part by the U. S. National Science Foundation.
[1] J. L. Yntema, Phys. Rev. **127**, 1659 (1962); **131**, 811 (1963).
[2] E. Rost, B. F. Bayman, and R. Sherr, Bull. Am. Phys. Soc. **9**, 458 (1964).
[3] R. Sherr, E. Rost, and M. Rickey, Phys. Rev. Letters **12**, 420 (1964).

discuss is the (d,p) reaction among spinless "nucleons." Then in zero-range distorted-waves approximation, after having made all the customary simplifications of the reaction mechanism, the amplitude for this stripping reaction takes the form

$$T=\text{const}\times\int\chi_p^{(-)*}(\mathbf{r}_1)\xi_{AB}^*(\mathbf{r}_1)\chi_D^{(+)}(\mathbf{r}_1)d^3r_1, \quad (1)$$

where

$$\xi_{AB}^*(\mathbf{r}_1)=\int\Phi_B^*(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\cdots)\times\Phi_A(\mathbf{r}_2,\mathbf{r}_3,\cdots)d^3r_2d^3r_3\cdots. \quad (2)$$

Here $\chi_p^{(-)}$ and $\chi_D^{(+)}$ are the distorted waves for the proton and deuteron, respectively. These functions are fully determined by the optical potentials and energies for the particles in question, and will receive no further discussion in the present paper. The wave functions Φ_A and Φ_B are the eigenfunctions for the target nucleus and product nucleus, respectively. To characterize these, say for Φ_A, we introduce the binding energy E_A, the angular momentum quantum numbers L_A and M_A, and any other necessary quantum numbers α_A. Then the stripping amplitude makes use of the overlap $\xi_{AB}(\mathbf{r})$ between the two bound nuclear wave functions Φ_A and Φ_B. The present paper concerns methods of construction of $\xi_{AB}(\mathbf{r})$. Evidently this is a problem in nuclear structure, and no very general solutions of this problem are to be expected.

The function $\xi_{AB}(\mathbf{r})$ often is called the "wave function of the captured neutron." It is also known as the "form factor" of the reaction. Understanding of this form factor is gained by making appropriate series expansions of the wave functions Φ_A and Φ_B. However, one expansion which it is interesting to consider first is the expansion in angular momentum of $\xi_{AB}(\mathbf{r})$ itself. Thus

$$\xi_{AB}(\mathbf{r})=\textstyle\sum_l\xi_{AB}^{(l)}(\mathbf{r})\,. \quad (3)$$

Here $L_A+L_B\geqslant l\geqslant|L_A-L_B|$ and the values of l are either all odd or all even, as governed by the parity of the transition. The expansion (3) has the well-known property that terms corresponding to different l yield contributions which do not interfere when the differential cross section is computed. Therefore, the cross section always separates into partial cross sections which are characterized by l. Often only one l value is important. In any case, we are free to concentrate attention upon a single l value.

Authors usually consider that the partial form factor $\xi_{AB}^{(l)}$ corresponds very closely to the wave function of the nearest single-particle state of the shell model, which has the angular momentum in question. If A is a closed-shell nucleus this correspondence often is almost inescapable. However, as the situation becomes more complicated we find two new effects: (a) The nearby state of angular momentum l becomes fragmented among several states Φ_B of the residual nucleus having different energies and (b) distant single-particle states which have angular momentum l must be considered. In fact effects (a) and (b) are related, and this relationship affects the radial shapes of the partial form factors.

We see in Eq. (1) that the radial shape of the partial form factor controls its overlap with the distorted waves. Because the distorted waves tend not to penetrate to the nuclear interior, this overlap tends to be best at radii near and somewhat outside of the "nuclear surface" region, and we must construct $\xi_{AB}^{(l)}$ which are as accurate as possible at such radii.[4] There is some simplification because at *asymptotically* large radii the shape of $\xi_{AB}^{(l)}$ is determined by the reaction Q, so that only the normalization must be found. Nevertheless experience[5] with the integral of Eq. (1) shows that asymptotic radii do not dominate the overlap, so that the importance of Q must not be overstressed.

Until recently most of the more accurate stripping calculations have constructed $\xi_{AB}^{(l)}$ as an eigenfunction in a single-particle (s.p.) well whose depth is adjusted to make the eigenenergy equal to (E_B-E_A), i.e., to fit the Q. By using this phenomenological procedure the asymptotic tail of the form factor is fitted to have a correct shape. If a given shell model state should be fragmented among several states Φ_B, then this procedure for constructing form factors forces the various partial form factors to have different shapes. Evidently admixing of distant single-particle states, effects of type (b), is implied by this procedure.

The present paper considers the question of how configuration splitting is related to the mixing in of distant states, and considers whether the phenomenological procedure which emphasizes the asymptotic tail of $\xi_{AB}^{(l)}$ does give a correct measure of the mixing which may be present. Other authors also are considering these questions,[1-3] and have already found that cross sections found by fitting the form factor to (E_B-E_A) often are severalfold different from those found by ignoring any dependence on E_B.

2. TWO EQUIVALENT NEUTRONS

We analyze first the simplest of all configuration splitting problems, the one which describes nucleus B as having two interacting neutrons in the l shell. It will be seen how the interaction of the neutrons mixes into the wave function s.p. states from higher shells, and it will be seen that the phenomenological procedure which fits form factors to reaction Q values probably gives a reasonably good picture of this mixing. Criticism of this analysis will be deferred until Sec. 3.

In the absence of interaction between the neutrons, each moves subject to the single-particle (s.p.) Hamiltonian

$$h(i)=K(i)+U(i)\,, \quad (4)$$

[4] This is why Gaussian bound-state wave functions are dangerous in reaction calculations.

[5] R. M. Drisko (private communication).

where K is the kinetic energy and U is the s.p. potential. The eigenfunctions of this h shall be written

$$h\phi_n=\epsilon_n\phi_n\,, \tag{5}$$

$$\phi_n=r^{-1}u_n(r)Y_{lm}(\hat{r})\,. \tag{6}$$

(Here, as henceforth, the quantum numbers l,m are suppressed except where they are needed explicitly. All s.p. wave functions used in this section will have angular momentum l.)

Nucleus A is assumed to have just one neutron outside a closed shell; hence Φ_A is a member of the set ϕ_n. For simplicity we suppose

$$\Phi_A=\phi_0\,,\quad E_A=\epsilon_0\,. \tag{7}$$

Nucleus B has two interacting neutrons of angular momentum l; hence Φ_B satisfies the Schrödinger equation

$$\{h(1)+h(2)+v(1,2)-E_B\}\Phi_B(l^2,E_BL_BM_B)=0\,, \tag{8}$$

where $v(1,2)$ is the interaction. Here the quantum numbers which label Φ_B are indicated, but the coordinates $\mathbf{r}_1$, $\mathbf{r}_2$ are omitted. Evidently if Φ_B is constructed from two particles having angular momentum l then it must be of the form

$$\Phi_B=r_1^{-1}r_2^{-1}w_B(r_1)w_B(r_2)\,|l^2,\,L_BM_B\rangle\,. \tag{9}$$

The ket denotes the vector-coupled product of two spherical harmonics Y_l. The two radial functions in Eq. (9) are identical because the neutrons are identical. (Antisymmetrization is accomplished by selecting either all odd values of L_B, or all even values.) Evidently there is no reason why $w_B(r)$ of Eq. (9) should be the same as $u_0(r)$ of the uncoupled problem. Furthermore it must be expected that each different one of the states L_B into which the l^2 configuration splits will have a different radial function w_B.

In standard shell-model calculations the energies E_B, belonging to each L_B, are found by using u_0 for w_B in Eq. (9) and calculating the expectation of the Hamiltonian operator. The result is

$$E_B\approx 2\epsilon_0+\langle 00,L_B|\,v\,|00,L_B\rangle\,, \tag{10}$$

where $|00,L_B\rangle$ denotes two functions ϕ_0 coupled up to angular momentum L_B. Equation (10) uses the zero-order wave function, as we expect for the energy in first-order perturbation theory. However, stripping theory requires more accurate knowledge of the wave function $w_B(r)$. If this function is expressed as a series in the set u_n,

$$w_B(r)=\sum_{n=0}^{\infty}a_{Bn}u_n(r)\,, \tag{11}$$

then up to first order it is

$$w_B(r)=u_0(r)+\sum_{n=1}^{\infty}(\epsilon_0-\epsilon_n)^{-1}u_n(r)\times\langle 0n,L_B|\,v\,|00,L_B\rangle\,. \tag{12}$$

Here $|0n,L_B\rangle$ denotes the coupling up to L_B of two s.p. functions ϕ_0 and ϕ_n.

The stripping form factor is found by inserting Eqs. (7) and (9) into Eq. (2). To first order the result is

$$\xi_{AB}{}^{(l)}(\mathbf{r})=r^{-1}w_B(r)Y_{lm}(\hat{r})\,, \tag{13}$$

where Eq. (12) is used for $w_l(r)$. Equation (13) will be regarded as the "exact" result, with which the phenomenological procedure for constructing the form factor will be compared.

Some interpretation of Eq. (12) is achieved if we view Eq. (9) as a trial wave function for a variational calculation of Φ_B. The Euler-Lagrange equation which the function w_B satisfies then is an elementary Hartree-Fock equation, in which the self-consistent single-particle potential depends upon the value of L_B. The self-consistent s.p. potential in which a neutron moves then is found to be

$$U_{\mathrm{SC}}(1)=U(1)+\int_0^{\infty}[w_B(2)]^2\times\langle l^2,L_B|\,v(1,2)\,|l^2,L_B\rangle dr_2\,. \tag{14}$$

The bra-ket expression indicates the angular integrations over the interaction $v(1,2)$. The self-consistent potential changes as we go from one state to another of the split configuration. This change gives to the radial wave functions tails which are consistent with the eigenenergies E_B, and controls other aspects of their radial shapes. Further application of the ideas that lead to Eq. (14) will be made in Sec. 3.

The customary phenomenological approximation for $\xi_{AB}{}^{(l)}(\mathbf{r})$ may now be discussed and compared with the expression found above. This approximation makes use of E_B, the *measured energy* of the state of the product nucleus which is formed. In the present analysis Eq. (10) is this "measured energy." Then in the phenomenological procedure the function used in Eq. (13) in place of $w_B(r)$ is $w_B'(r)$, and $w_B'(r)$ is fitted to the measured energy. The procedure is governed by the equations

$$\phi_B'(\mathbf{r})=r^{-1}w_B'(r)Y_{lm}\,, \tag{15}$$

$$h_B'\phi_B'(\mathbf{r})=(E_B-\epsilon_0)\phi_B'(\mathbf{r})\,, \tag{16}$$

$$h_B'\equiv K+\lambda_BU=h+(\lambda_B-1)U\,, \tag{17}$$

so that

$$\Phi_B\approx r_1^{-1}r_2^{-1}w_B'(r_1)u_0(r_2)\,|l^2,L_BM_B\rangle\,. \tag{18}$$

It is seen that the depth of the s.p. potential is adjusted so that the imitation s.p. state ϕ_B' has an energy which is just sufficient to make up the measured energy E_B

as a sum of s.p. energies. The interaction is not carried Then it is easy to solve for w_B' up to first order in the perturbation $(\lambda_B-1)U$ and to substitute out λ_B in terms of E_B. The result is

$$w_B'(r)\approx u_0(r)+\langle 00,L_B|v|00,L_B\rangle\langle 0|U|0\rangle^{-1} \times\sum_{n=1}^{\infty}(\epsilon_0-\epsilon_n)^{-1}\langle n|U|0\rangle u_n(r)\,. \quad (19)$$

Equation (19) must be compared with Eq. (12) in order to assess the accuracy of the phenomenological procedure.

Equations (12) and (19) would be exactly equivalent if the ratio

$$\langle n0,L_B|v|00,L_B\rangle/\langle n|U|0\rangle \quad (20)$$

were independent of n. In this circumstance the correction to the s.p. potential in Eq. (17) would be of *the same shape* as the self-consistent correction term in Eq. (14). Evidently if the shapes of these two corrections should be the same, then the procedure of fitting to E_B would guarantee a correct value of the over-all magnitude of the correction term in the wave function in Eq. (19). This analysis leads to two observations regarding the accuracy of the phenomenological procedure. The first observation is an optimistic one, that at least the phenomenological procedure does not appear to give a grossly wrong estimate of the admixture in the wave function. The second observation concerns the deficiencies which are found if the procedure is studied more carefully. The correction term in Eq. (14) probably has the shape of the s.p. wave function $[u_0(r)]^2$, and is likely to be peaked at the nuclear surface. The correction term in Eq. (17), on the other hand, has the shape of the s.p. potential, $U(r)$, itself. Thus the two corrections may well exhibit admixtures which differ in detail.

3. DISCUSSION

The elementary configuration splitting problem of Sec. 2, wherein nucleus B has just two interacting neutrons in the l shell, is a sufficient indicator of the physical effects which must be considered, to permit us to discuss all other cases by comparison with this case.

What was found for the two-neutron case was that the phenomenological procedure of fitting the form factor to the reaction Q introduces into the single-particle wave function about the same amount of admixture of higher states as a nuclear structure calculation had indicated to be present. The two methods may not give identical estimates for the shape of the admixture, but this may be regarded, for the moment, as a secondary question. (Of course, the two shapes do agree identically at asymptotically large radii.) However, the reason why the admixture in any one state Φ_B could be tied to the energy shift for this state was that the coupling scheme for the state Φ_B could be specified in advance of the calculation. As a result there was no more freedom in the nuclear structure calculation for two particles than there is in the model problem (particle+core), which is the dynamical basis of the phenomenological method.

In general, the state Φ_B may be expanded in a complete set of eigenstates of nucleus A coupled together with a complete set of s.p. states for particle 1. This is the parentage expansion:

$$\Phi_B(E_B,\alpha_B L_B M_B)=\sum_{A',n,l}\{\phi_{nl}(1),\Phi_{A'}\}_{L_B M_B} \times[(nl,A')L_B\|\alpha_B L_B]\,. \quad (21)$$

In the two-particle case the sum over A' and l collapses to only one term, and then the sum over n factors out as an alteration of only the radial function of ϕ_{0l}. This factorization yields the approximate agreement with the phenomenological method.

If nucleus B has more than two particles outside the closed-shell core, then a state Φ_B is likely to have a variety of parent states, having different A' and l, and the series (21) will have more than one term which is nonvanishing. As a result no factorization of Φ_B is possible, and the close relation between the stripping form factor and the energy of state Φ_B is lost. Equation (2) prescribes how to calculate the form factor, and it is

$$\xi_{AB}(\mathbf{r}_1)=\sum_{n,l,m}\phi_{nlm}(\mathbf{r}_1)\langle lL_A,mM_A|L_B M_B\rangle \times[(nl,A)L_B\|\alpha_B L_B]\,, \quad (22)$$

so that the partial form factor is

$$\xi_{AB}{}^{(l)}(\mathbf{r}_1)=\sum_{n,m}\phi_{nlm}(\mathbf{r}_1)\langle lL_A,mM_A|L_B M_B\rangle \times[(nl,A)L_B\|\alpha_B L_B]\,. \quad (23)$$

Thus the partial form factor, which determines the stripping cross section for angular momentum transfer l, is obtained from just one term of the complicated wave function Φ_B. The energy E_B, on the other hand, is obtained only by use of all terms in the expansion (21) of Φ_B. Indeed, cross terms are likely to be of special importance in calculating the energy. In this situation it is quite wrong to use the energy E_B to measure the radial shape of only the one term, Eq. (23), which comes out of the expansion (21). In other words, as soon as the parentage expansion becomes nontrivial, the phenomenological procedure becomes incorrect.

Even the treatment of the two-particle problem was a little oversimplified, and this case is not quite so much easier than the many-particle problem as is suggested above. Correlation of the two nucleons actually mixes in with the product wave function of Eq. (9) terms built from s.p. states that have angular momenta different from l, and also terms in which the radial motions of the two particles are coupled. However, such effects probably lie entirely outside of a shell model context and must be disregarded in the present analysis.

What is of greatest interest is the question of how to construct form factors which are sufficiently accurate for practical stripping calculations. The phenomenological procedure of fitting an imitation single-particle state to the measured energy of Φ_B is at least straightforward, and it does fit the shape of the asymptotic tail of the form factor. However, while variation of the value of E_B to which we fit does not drastically affect the angular distribution which is predicted, it is known[6] that such variation affects the magnitude of the cross section by about 30% per 1-MeV change of E_B. Thus if Φ_B is a mixture of several terms, and we wish to use stripping theory to measure from experiment the amplitude with which each term appears, then uncertainty in the *shape* of the partial form factor for each term can lead to large uncertainty about its magnitude.

No easy prescription for calculating radial shapes of form factors is possible, and this must instead be regarded as a general subject of nuclear structure analysis. Probably no analysis will ever yield a reliable procedure for handling the small components of Φ_B. For the major components of Φ_B, derived from one or two nearby shell-model configurations, the correct shape of each form factor probably lies somewhere between two extreme possibilities: either (a) the shape calculated in terms of E_B by the phenomenological procedure or (b) the shape calculated from the energy of the unsplit configuration from which that component was derived. Of course procedure (b) would require a knowledge of "single-particle energies" before form factors could be computed. Because these energies are, in turn, derived from stripping experiments, a complete analysis of any one experiment would then require some juggling of these energies, in order to achieve self-consistency. Whether procedure (a) or procedure (b) is closer to the truth depends on whether the radial integration in Eq. (1) is dominated by values of r_1 which are largely outside the nucleus or whether contributions from a little inside the nucleus may be important.

Some indication can be given of how to calculate improved form factors from a more basic point of view than just described. Equation (21) expresses Φ_B as a sum over A', n, and l. Normal nuclear structure calculations do not carry the sum over n. What this sum expresses is the improvement of the shape of the single-particle radial wave function that goes with each value of A' and l. Thus this sum is decisive for the calculation of partial form factors, as is seen in Eq. (23). However, it was observed earlier in the two-particle case [see Eq. (14)] that a correct radial wave function could be computed directly, without any sum over n, by the artifice of constructing a self-consistent single-particle potential in which the coupling of particle 1 with the rest of the nucleus is incorporated. The self-consistent potential may be constructed with sufficient accuracy with the use of only the shell-model wave function for Φ_B, in which the sum over n is omitted. Then the correct form factor is computed as an eigenfunction in the self-consistent potential. The generalization of this method for Φ_B states that have more than two particles is straightforward. G. R. Satchler and W. T. Pinkston have been conducting some calculations which employ this method.[7]

The question of the proper determination of radial wave functions, the subject of this paper, comes up in many applications. The bound-state single-particle wave functions which are used for nuclear structure calculations are designed to be at their best in the nuclear interior, where interactions among nucleons are strong. These wave functions are not correct in the region of the nuclear surface, and must be improved if effects which take place in the surface region are to be calculated. An interesting example in which such an improvement is required comes up in the theory of the E1 giant resonance.[8] After diagonalizing the shell-model Hamiltonian the final states formed by E1 absorption are found to lie in the continuum, and far above the energies of the unsplit shell-model configurations from which they are formed. In order to calculate the decay widths of these states it is necessary to improve their radial wave functions,[9] in just the fashion discussed in the present article. Here again it might be satisfactory to find the decay widths by calculating single-particle states in a self-consistent s.p. potential which is adapted to the giant resonance.

ACKNOWLEDGMENTS

The author wishes to acknowledge the hospitality of the Physics Division of the Aspen Institute for Humanistic Studies during June-July 1963, where the major part of this work was performed. He also wishes to acknowledge some correspondence with E. S. Rost and G. R. Satchler, and also the receipt of prepublication copies of the articles by Dr. Rost and his collaborators. Conversations with E. U. Baranger, B. L. Cohen, R. M. Drisko, and R. A. Sorenson were very helpful for the preparation of a more orderly paper.

[6] B. L. Cohen, R. E. Price, and S. Mayo, Nucl. Phys. **20**, 370 (1960).

[7] G. R. Satchler (private communication).

[8] G. E. Brown and M. Bolsterli, Phys. Rev. Letters **3**, 472 (1959).

[9] M. Bauer, Ph.D. thesis, University of Maryland, 1962 (unpublished).