

funktionen selbst kann also allenfalls darin gesehen werden, daß die ersten beiden Koeffizienten in (1) ungefähr gleich dem arithmetischen Mittel der Koeffizienten in Tab. 3 sind.

Vergleicht man dagegen bei den nach den beiden Methoden bestimmten Zustandsfunktionen die Elektronendichte im 3-dimensionalen Raum, so findet man nur geringfügige Unterschiede. Als Beleg dafür ist in der Abb. 6 die Elektronendichte längs der Kernverbindungsline gezeichnet, und zwar in gestrichelten Kurven für die Ransil-Funktion, in ausgezogenen Kurven für ψ_b und nur durch einige Kreuze angedeutet für ψ_a . Obgleich nun die Abbildungen für das Dichte„plateau“ um die Molekül-

mitte deutlich einen höheren Wert bei der Ransil-Funktion zeigen, ist doch die Folgerung zu ziehen, daß die drei Funktionen ψ_{Ransil} , ψ_a , ψ_b in diesem Gebiet zu fast gleicher Dichte führen würden, wenn die Kernabstände gleich wären; denn bei der Verkürzung des Abstands von 5,224 und 5,051 ist natürlich eine Erhöhung der Dichte um den Faktor $(5,224/5,051)^3$, d. h. um 11% zu erwarten. Nur der über diese 11% hinausgehende Unterschied zwischen den Dichten ist also als echter Unterschied anzusehen. Er ist sehr klein und rührt her von der Gleichheit der Koeffizienten für homöopolare und ionische Anteile und dem Aufbrechen der K-Schale bei der Ransilschen Zustandsfunktion.

Treatment of Cluster Channels in Nuclear Reactions above the Two-Particle Threshold *

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Within the framework of the eigenchannel reaction theory above the two-particle threshold cluster channels are introduced. The eigenchannels of the S -matrix are used, i. e. continuum states which diagonalize both the S -matrix and the nuclear Hamiltonian and represent for each reaction energy a discrete set of coupled channel wave functions with a common (eigen-) phase. Especially the emission of a deuteron is discussed. It is shown that the cluster channels supplement the energy-correlated channels describing the energy partition $\varepsilon_1 + \varepsilon_2 = E - E_f$ and that asymptotic channel orthogonality holds. The characteristic feature of the cluster channels as compared to the energy-correlated channels is that their final state interaction is not limited to a finite matching volume comparable to nuclear sizes.

In nuclear reactions above the two-particle threshold one has to consider several types of two-, and many-particle channels besides the one-particle channels which are characterized by the escape of one, two or several particles into the continuum. The emission of two non-interacting, i. e. free, nucleons of momenta k_1 , k_2 with fixed energy $k^2 = k_1^2 + k_2^2$ represents a limiting case of two energy-correlated particles whose final state interaction occurs in a region (and reaction time) comparable to the size of the nuclear compound system.

At a given total channel energy E of the compound A -particles system the energies ε_1 , ε_2 of the

two emitted particles are continuous in the range

$$\varepsilon_1 + \varepsilon_2 = E - E_f, \quad (1)$$

where E_f denotes the final energy of the residual $(A-2)$ particle system.

This characteristic energy partition can be described, as shown in ref. ¹ and independently in ref. ², by introducing suitable coordinates. If the emitted particles are detected at asymptotic distances r_1 and r_2 from the compound nucleus (target) so that the lifetime of the excited compound state involved in this particular two-particle emission channel becomes extremely small compared to their

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¹ L. M. DELVES, Nucl. Phys. **9**, 391 [1959] ; **20**, 275 [1960]. — N. F. MOTT and H. S.W. MASSEY, The Theory of Atomic Collisions, Clarendon Press, Oxford 1965, Ch. XIV, p. 399.

² M. DANOS and W. GREINER, Z. Phys. **202**, 125 [1967].



common time of flight t , then

$$r_1/r_2 = v_1/v_2 = (\varepsilon_1/\varepsilon_2)^{\frac{1}{2}}. \quad (2)$$

In other words, $\alpha = \arccot(r_1/r_2)$ defines the (asymptotic) energy-correlation angle of the two emitted particles.

Besides these quasi-free two- and many-particle channels a bound system of several nucleons can be emitted. These continuum channels are called cluster channels, and correspond to a discrete set of energy partitions of the available total channel energy E ,

$$E = E_f + (E_{CM} - |E_B|), \quad (3)$$

where E_{CM} denotes the center-of-mass energy and E_B the binding energy of the cluster. Then the only two-particle cluster channels are outgoing deuterons on which we concentrate.

The characteristic feature of such cluster channels is the fact that their final state interaction extends to the asymptotic region.

The objective of this paper is to introduce the cluster channels and show that asymptotic channel orthogonality holds for the cluster and energy-correlated channel wave functions. Numerical estimates are given for the overlap of two channel wave functions depending on the center-of-mass distance of the cluster from the target nucleus which is supposed to be heavy compared to the emitted particles.

We use the eigenchannel reaction theory³ as an extension of the bound-state particle-hole shell model to describe in general terms the solution of the nuclear Hamiltonian including the continuum. The essential procedure of this shell model version of reaction theory is that one constructs solutions of the nuclear Hamiltonian in the continuum which are also eigenfunctions of the S -matrix. This is achieved by dividing the physical space into an inside and an outside region and imposing natural boundary conditions on the discrete inside solutions.

Due to the boundary condition only those energy-correlated two-particle channels can be taken into account whose final state interaction is confined to an internal region of the order of 5 to 20 times the nuclear size. In other words, one adopts as basis states for the energy-correlated outgoing pairs of nucleons only those channel wave functions^{1, 2, 4}

$$d_{\frac{1}{2}(l_1+l_2+1), \frac{1}{2}(l_1-l_2)}^{n+\frac{1}{2}(l_1+l_2+1)}(2\alpha)$$

of the few lowest quantum numbers n, l_1, l_2 .

³ M. DANOS and W. GREINER, Phys. Rev. **133**, B 93 [1965]; **146**, 708 [1966].

Here we treat explicitly cluster channels. These channels are contained in the energy-correlated basis. However, they correspond to superpositions of energy-correlated wave functions with large quantum number n . The motive to introduce in addition this cluster basis is, of course, to keep the effective approximate configuration space small, i. e. to diagonalize small energy matrices. We have to pay for this approach which explicitly includes the most important experimental channels by the fact that the cluster channel and the correlated two-particle channel wave functions are no more strictly orthogonal. Therefore, one problem studied here is the asymptotic orthogonality between cluster and correlated two-particle channels. From the numerical estimate of the orthogonality overlap integral depending on the center-of-mass distance of the cluster from the residual nucleus it is found that orthogonality can be practically achieved if the inside (interaction) region is chosen large enough.

In this paper it is assumed that all processes take place at non-relativistic energies so that one can properly treat the center-of-mass motion by eliminating the spurious states through a diagonalization of the center-of-mass Hamiltonian.

In Section I the energy-correlated two-particle channels are reviewed and the correlations involved are studied while in the second section the cluster channel wave functions are defined. In Section III the channel orthogonality is investigated and a practical method to solve the nuclear Hamiltonian in the internal region is suggested in Section IV.

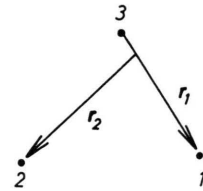


Fig. 1. Relative coordinates for a three-particle channel, the residual nucleus 3 and two light emitted particles 1 and 2.

I. Energy-Correlated Channels

For a two-particle emission channel only the total energy E_α is specified. In terms of the relative and

⁴ P. M. MORSE and H. FESHACH, Methods of Theoretical Physics, McGraw-Hill, New York 1953, Ch. 12.3, p. 1731.

center-of-mass coordinates for the 3-body system, viz.

$$\begin{aligned}\mathbf{r}_1 &= \mathbf{r}_{p1} - \mathbf{r}_{p3}, \\ \mathbf{r}_2 &= \mathbf{r}_{p2} - \frac{m_1}{m_1+m_3} \mathbf{r}_{p1} - \frac{m_3}{m_1+m_3} \mathbf{r}_{p3}, \\ \mathbf{R} &= \frac{m_1 \mathbf{r}_{p1} + m_2 \mathbf{r}_{p2} + m_3 \mathbf{r}_{p3}}{m_1+m_2+m_3},\end{aligned}\quad (4)$$

the Schrödinger equation at asymptotic distance from the target nucleus (labeled 3 in Fig. 1), i. e. in the force-free region, is the sum of kinetic energies,

$$\left(-\frac{\hbar^2}{2\mu_1} \nabla^2(\mathbf{r}_1) - \frac{\hbar^2}{2\mu_2} \nabla^2(\mathbf{r}_2) - E_a\right) R(\mathbf{r}_1, \mathbf{r}_2) = 0, \quad (5)$$

with the reduced masses

$$\begin{aligned}\mu_1 &= m_1 m_3 / (m_1 + m_3), \\ \mu_2 &= m_2 (m_1 + m_3) / (m_1 + m_2 + m_3)\end{aligned}\quad (6)$$

and the channel energy

$$E_a = \hbar^2 k_1^2 / (2\mu_1) + \hbar^2 k_2^2 / (2\mu_2). \quad (7)$$

Let us assume that the target or residual nucleus 3 is heavy compared to the two emitted particles. Then $\mu_1 = m_1$ and $\mu_2 = m_2$. Furthermore, \mathbf{r}_1 and \mathbf{r}_2 represent the distance of particles 1 and 2 from the residual nucleus 3, respectively. The uncorrelated

product wave functions $\varphi(\mathbf{r}_1, \mathbf{r}_2)$ of

$$(\nabla^2(\mathbf{r}_1) + \nabla^2(\mathbf{r}_2) + k_1^2 + k_2^2) \varphi(\mathbf{r}_1, \mathbf{r}_2) = 0 \quad (8)$$

with sharp particle energies k_1^2, k_2^2 do not represent a suitable basis because only the total channel energy $E_a = E - E_t$ is sharp. An expansion of the scattering matrix in terms of these single-particle wave functions with sharp energies would require a continuum of channels. Experimentally one measures a probability distribution associated with the continuous energy partition among the two emitted particles suggesting to describe the energy partition by suitable coordinates either in the coordinate or in the momentum space.

For simplicity let us consider the emission of two light particles of equal mass, $m_1 = m_2$. Using the energy-correlation angle α defined by

$$r_1 = r \cos \alpha, \quad r_2 = r \sin \alpha \quad (9)$$

so that asymptotically

$$r_1/r_2 = v_1/v_2 = \sqrt{\varepsilon_1/\varepsilon_2} = \text{const}$$

holds, Eq. (5) separates into a radial equation⁴

$$\left[\frac{1}{r^5} \frac{d}{dr} \left(r^5 \frac{d}{dr} \right) + k^2 - \frac{1}{r^2} ((l_1 + l_2 + 2n + 2)^2 - 4) \right] R(r) = 0 \quad (10)$$

(l_1, l_2, n)	$2 \left(\frac{2n + l_1 + l_2 + 2}{\sin 2\alpha} \right)^{\frac{1}{2}} a_{\frac{1}{2}(l_1 + l_2 + 1), \frac{1}{2}(l_1 - l_2)}^{(\frac{1}{2}(l_1 + l_2 + 1) + n)}(2\alpha)$
$(0, 0, n)$	$\frac{4}{\sqrt{\pi}} \frac{\sin 2(n+1)\alpha}{\sin 2\alpha}$
$(0, 1, n)$	$2 \left(\frac{(n+1)\pi}{n+2} \right)^{\frac{1}{2}} \frac{1}{\sin \alpha \sin 2\alpha} \left[\sin 2(n+1)\alpha - \frac{n+1}{n+2} \sin 2(n+2)\alpha \right]$
$(0, 2, n)$	$\left(\frac{n+3}{(n+\frac{5}{2})(n+\frac{3}{2})(n+1)\pi} \right)^{\frac{1}{2}} \frac{1}{\sin^2 \alpha \sin 2\alpha} \left[(n+\frac{5}{2}) \sin 2(n+1)\alpha - 2(n+1) \sin 2(n+2)\alpha \right. \\ \left. + \frac{(n+1)(2n+3)}{2(n+3)} \sin 2(n+3)\alpha \right]$
$(1, 2, n)$	$\frac{1}{4} \left(\frac{(n+4)(n+3)}{(n+2)(n+1)\pi} \right)^{\frac{1}{2}} \frac{1}{\sin^3 \alpha \cos^2 \alpha} \left[\sin 2(n+1)\alpha - \frac{n+1}{n+3} \sin 2(n+2)\alpha \right. \\ \left. - \frac{n+1}{n+3} \sin 2(n+3)\alpha + \frac{(n+1)(n+2)}{(n+3)(n+4)} \sin 2(n+4)\alpha \right]$
$(l_1, l_2, 0)$	$\left(\frac{2\Gamma(l_1 + l_2 + 3)}{\Gamma(l_1 + \frac{3}{2})\Gamma(l_2 + \frac{3}{2})} \right)^{\frac{1}{2}} (\cos \alpha)^{l_1} (\sin \alpha)^{l_2}$
$(l_1, l_2, 1)$	$\left(\frac{\Gamma(l_1 + l_2 + 3)\Gamma(l_1 + l_2 + 4)}{2\Gamma(l_1 + \frac{3}{2})\Gamma(l_2 + \frac{3}{2})} \right)^{\frac{1}{2}} (\cos \alpha)^{l_1} (\sin \alpha)^{l_2} [2l_2 + 3 - 2(l_1 + l_2 + 3) \sin^2 \alpha]$
$(l_1, l_2, 2)$	$\frac{1}{4} \left(\frac{(l_1 + l_2 + 6)\Gamma(l_1 + l_2 + 4)}{2\Gamma(l_1 + \frac{3}{2})\Gamma(l_2 + \frac{3}{2})} \right)^{\frac{1}{2}} (\cos \alpha)^{l_1} (\sin \alpha)^{l_2} [(2l_2 + 5)(2l_2 + 3) - 4(l_1 + l_2 + 4) \\ \cdot (2l_2 + 5) \sin^2 \alpha + 4(l_1 + l_2 + 5)(l_1 + l_2 + 4) \sin^4 \alpha]$

Table of Energy Correlated Channel Wave Functions.

whose regular and irregular solutions $R(r)$ are Bessel and Neumann functions

$$r^{-2} J_{l_1+l_2+2n+2}(kr) \quad \text{and} \quad r^{-2} N_{l_1+l_2+2n+2}(kr) \quad (11)$$

with

$$n = 0, 1, 2, \dots$$

and an energy-correlation equation

$$\left\{ \frac{4}{\sin^2 2\alpha} \frac{d}{d\alpha} \left(\frac{1}{4} \sin^2 2\alpha \frac{d}{d\alpha} \right) - \left(\frac{l_1(l_1+1)}{\cos^2 \alpha} + \frac{l_2(l_2+1)}{\sin^2 \alpha} \right) + (l_1+l_2+2n) \cdot (l_1+l_2+2n+4) \right\} A(\alpha) = 0 \quad (12)$$

with the solutions

$$A_{l_1 l_2 n}(\alpha) = (\sin 2\alpha)^{-\frac{1}{2}} d_{\frac{1}{2}(l_1+l_2+1), \frac{1}{2}(l_1-l_2)}^{\frac{1}{2}(l_1+l_2+1)+n} (2\alpha) \quad (13)$$

where l_1 and l_2 denote the angular momenta of the two particles. These energy-correlation components $A_{l_1 l_2 n}(\alpha)$ of the complete channel wave function are given in Table 1 for a selection of quantum numbers (l_1, l_2, n) .

The continuous energy spectrum of the two emitted particles associated with the angle α defining the sharp energy partition, in other words the cross section of particle pairs emitted with the energy partition between α and $\alpha + d\alpha$, is proportional to

$$\left(d_{\frac{1}{2}(l_1+l_2+1), \frac{1}{2}(l_1-l_2)}^{\frac{1}{2}(l_1+l_2+1)+n} (2\alpha) \right)^2 \sin 2\alpha d\alpha. \quad (14)$$

In particular for $n=0$ the energy-correlation wave $A_{l_1 l_2 0}(\alpha)$ is proportional to (see Table 1)

$$(\cos \alpha)^{l_1} (\sin \alpha)^{l_2}$$

exhibiting precisely one maximum in the energy spectrum at $\tan \alpha = \sqrt{l_2/l_1}$ which moves toward $\alpha=0$ for $l_1 \gg l_2$ and $\alpha=\pi/2$ for $l_2 \gg l_1$. For $n=1$ and arbitrary angular momenta l_1, l_2 there are two maxima etc., indicating that one can read off an experimental spectrum the maximum channel quantum number n involved.

On introducing the radial wave function $u(r)$ instead of

$$R(r) = r^{-5/2} u(r) \quad (15)$$

and the energy-correlation wave function $D(\alpha)$ instead of

$$\sqrt{\frac{2n+l_1+l_2+2}{\sin 2\alpha}} d_{\frac{1}{2}(l_1+l_2+1), \frac{1}{2}(l_1-l_2)}^{\frac{1}{2}(l_1+l_2+1)+n} (2\alpha) = \frac{D(\alpha)}{\sin \alpha \cos \alpha} \quad (16)$$

the radial and energy partition Eqs. (10), (12) transform into

$$\left(-\frac{d^2}{dr^2} + \frac{(l_1+l_2+2n+\frac{3}{2})(l_1+l_2+2n+\frac{5}{2})}{r^2} - k^2 \right) u(r) = 0 \quad (17)$$

and

$$\left(-\frac{d^2}{d\alpha^2} + \frac{l_1(l_1+1)}{\cos^2 \alpha} + \frac{l_2(l_2+1)}{\sin^2 \alpha} - (l_1+l_2+2n+2)^2 \right) D(\alpha) = 0. \quad (18)$$

From Eq. (17) it is obvious that the channel index $l = l_1 + l_2 + 2n + \frac{3}{2}$ plays the role of a generalized angular momentum. In particular, it enforces a node of the order $l + \frac{5}{2}$ on the radial wave function at $r=0$ so that high channel indices are suppressed at given energy k^2 for small pair impact parameters. Likewise the angular momenta l_1, l_2 in Eq. (18) enforce nodes of the orders l_1 and l_2 at $\alpha=\pi/2$ and $\alpha=0$, respectively, on the energy partition component of the channel wave function.

The lowering and raising operators associated with the symmetric projection quantum number $\frac{1}{2}(l_1+l_2+1)$ are obtained by factorization of Eq. (18), yielding

$$P_{\pm} = (l_1+l_2) \cot 2\alpha + \frac{l_2-l_1}{\sin 2\alpha} \mp \frac{d}{d\alpha} \quad (19)$$

and

$$P_+ P_- = -\frac{d^2}{d\alpha^2} + \frac{l_1(l_1+1)}{\cos^2 \alpha} + \frac{l_2(l_2+1)}{\sin^2 \alpha} - (l_1+l_2)^2.$$

The raising and lowering operators for the channel index are similarly obtained by factorization of Eq. (17),

$$C_{\pm} = \frac{l_1+l_2+2n+\frac{3}{2}}{r} \mp \frac{d}{dr}. \quad (20)$$

The channel wave functions

$$D(\alpha) [Y^{[l_1]}(\hat{r}_1) \times Y^{[l_2]}(\hat{r}_2)]_m^{[e]}$$

build up representations of $SO(6)$, and the raising and lowering operators are closely related to the generators of the Lie algebra of $SO(6)$ ^{5,6}.

The energy-correlation generator X_{α} corresponding to the coordinate α is obtained by transforming the two-particle wave function $\psi(\mathbf{r}_1, \mathbf{r}_2)$,

$$\begin{aligned} \psi(\mathbf{r}_1 + r \cos \alpha \hat{r}_1 d\alpha, \mathbf{r}_2 - r \sin \alpha \hat{r}_2 d\alpha) \\ = \psi(\mathbf{r}_1, \mathbf{r}_2) + (i/\hbar) d\alpha X_{\alpha} \psi(\mathbf{r}_1, \mathbf{r}_2) \end{aligned}$$

$$\text{where} \quad X_{\alpha} = r_2 \hat{r}_1 \cdot \mathbf{p}_1 - r_1 \hat{r}_2 \cdot \mathbf{p}_2 = \frac{\hbar}{i} \frac{\partial}{\partial \alpha} \quad (21)$$

so that X_{α} commutes with \mathbf{L}_1 and \mathbf{L}_2 .

The isotropic pair flux component is given by

$$\begin{aligned} j_p = \frac{\hbar}{2im} \left[\psi^*(\mathbf{r}_1, \mathbf{r}_2) \frac{\partial}{\partial r} \psi(\mathbf{r}_1, \mathbf{r}_2) \right. \\ \left. - \psi(\mathbf{r}_1, \mathbf{r}_2) \frac{\partial}{\partial r} \psi^*(\mathbf{r}_1, \mathbf{r}_2) \right] \end{aligned} \quad (22)$$

⁵ A. JOSEPH, Rev. Modern Phys. **39**, 829 [1967].

⁶ We use the notation of U. FANO and G. RACAH, Irreducible Tensorial Sets, Academic Press, Inc., New York 1959.

and yields as eigenvalue for the plane pair wave

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \exp[i \mathbf{k} \cdot \mathbf{r}] \cdot (\cos \alpha \cos \beta \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{r}}_1 + \sin \alpha \sin \beta \hat{\mathbf{k}}_2 \cdot \hat{\mathbf{r}}_2)$$

the pair velocity

$$v = (v_1^2 + v_2^2)^{\frac{1}{2}} \quad (23)$$

which is used to normalize the channel wave function to unit incoming pair flux.

The complete energy-correlated channel wave function of phase δ is, upon incorporating the normalization to incoming pair flux $v = (v_1^2 + v_2^2)^{\frac{1}{2}}$ per unit area into the radial wave, given by⁶

$$2 \sqrt{\frac{l_1 + l_2 + 2n + 2}{v \sin 2\alpha}} d_{\frac{1}{2}(l_1 + l_2 + 1), \frac{1}{2}(l_1 - l_2)}^{\frac{1}{2}(l_1 + l_2 + 1) + n} (2\alpha) \frac{1}{(kr)^2} [\cos \delta J_{l_1 + l_2 + 2n + 2}(kr) - \sin \delta N_{l_1 + l_2 + 2n + 2}(kr)] \times [Y^{[l_1]}(\hat{\mathbf{r}}_1) \times Y^{[l_2]}(\hat{\mathbf{r}})] \begin{matrix} [l] \\ m \end{matrix}. \quad (24)$$

The corresponding volume element is

$$d\tau = r_1^2 dr_1 d\hat{\mathbf{r}}_1 r_2^2 dr_2 d\hat{\mathbf{r}}_2 = r^2 \cos^2 \alpha d\hat{\mathbf{r}}_1 r^2 \sin^2 \alpha d\hat{\mathbf{r}}_2 r d\alpha dr = r^5 dr \frac{1}{4} \sin^2 2\alpha d\alpha d\hat{\mathbf{r}}_1 d\hat{\mathbf{r}}_2. \quad (25)$$

The natural boundary condition $\frac{\partial \ln \varphi}{\partial \ln r} \Big|_{r=c}$ for the radial part φ of the asymptotic wave function is formulated in terms of the distance $r = (r_1^2 + r_2^2)^{\frac{1}{2}}$ only².

In order to be able to apply shell model techniques of discrete states to the inner (interaction) region we incorporate into the effective Hilbert space in which the Hamiltonian is eventually diagonalized only those correlated two-particle channels whose final state interaction is limited to the interaction volume of the size of the single-particle matching radius. This restriction amounts to considering only the channels $\{l_1, l_2, l, m, n\}$ with the lowest few quantum numbers n and means essentially only those two-particle channels which besides the energy correlation $k_1^2 + k_2^2 = k^2$ are uncorrelated.

Since in the asymptotic region the proton and neutron in the deuteron cluster have the same distance from the residual nucleus (target) one has $r_1 = r_2$ or $\alpha = \pi/4$. One suspects, therefore, that the expectation value of $\sin^2 \alpha$ is $\frac{1}{2}$ for large correlated-channel quantum numbers n . This turns out to be true.

The orthogonality of the energy-correlated channel wave functions with respect to the quantum number n

$$\left(\frac{2n + l_1 + l_2 + 2}{\sin 2\alpha} \right)^{\frac{1}{2}} d_{\frac{1}{2}(l_1 + l_2 + 1), \frac{1}{2}(l_1 - l_2)}^{\frac{1}{2}(l_1 + l_2 + 1) + n} (2\alpha) = \left((2n + l_1 + l_2 + 2) \frac{\Gamma(n + l_1 + l_2 + 2) \Gamma(n + 1)}{\Gamma(n + l_1 + \frac{3}{2}) \Gamma(n + l_2 + \frac{3}{2})} \right)^{\frac{1}{2}} \cdot (\cos \alpha)^{l_1} (\sin \alpha)^{l_2} P_n^{(l_2 + \frac{1}{2}, l_1 + \frac{1}{2})}(\cos 2\alpha) \quad (26)$$

reduces to that of the Jacobi polynomials $P_n^{(\alpha, \beta)}(x)$ ⁷,

$$\int_{-1}^1 (1-x)^\alpha (1+x)^\beta P_n^{(\alpha, \beta)}(x) P_m^{(\alpha, \beta)}(x) dx = \delta_{nm} \frac{2^{\alpha+\beta+1}}{2n + \alpha + \beta + 1} \frac{\Gamma(n + \alpha + 1) \Gamma(n + \beta + 1)}{n! \Gamma(n + \alpha + \beta + 1)}. \quad (27)$$

Upon using the recurrence relation⁸

$$2(n+1)(n + \alpha + \beta + 1)(2n + \alpha + \beta) P_{n+1}^{(\alpha, \beta)}(x) = [(2n + \alpha + \beta + 1)(\alpha^2 - \beta^2) + x(2n + \alpha + \beta)(2n + \alpha + \beta + 1)(2n + \alpha + \beta - 2)] P_n^{(\alpha, \beta)}(x) - 2(n + \alpha)(n + \beta)(2n + \alpha + \beta + 2) P_{n-1}^{(\alpha, \beta)}(x), \quad (28)$$

the expectation value of $\sin^2 \alpha$ is

$$\langle \sin^2 \alpha \rangle_{l_1, l_2, n} = (2n + l_1 + l_2 + 2) \int_0^{2/\pi} [d_{\frac{1}{2}(l_1 + l_2 + 1), \frac{1}{2}(l_1 - l_2)}^{\frac{1}{2}(l_1 + l_2 + 1) + n} (2\alpha)]^2 \sin^2 \alpha \sin 2\alpha d\alpha = \frac{1}{2} \left[1 + \frac{(l_1 + l_2 + 1)(l_2 - l_1)(2n + l_1 + l_2 + 2)}{(2n + l_1 + l_2 + 1)(2n + l_1 + l_2 + 2)(2n + l_1 + l_2 + 3)} \right] = \frac{1}{2} + O(n^{-2}), \quad (29)$$

i. e. tends to $\frac{1}{2}$ as n goes to infinity.

⁷ One of the projection quantum numbers $\frac{1}{2}(l_1 + l_2 + 1)$ and $\frac{1}{2}(l_1 - l_2)$ of the energy-correlation channel wave function $d_{\frac{1}{2}(l_1 + l_2 + 1), \frac{1}{2}(l_1 - l_2)}^{\frac{1}{2}(l_1 + l_2 + 1) + n} (2\alpha)$ is always an integer while the other is a half-integer.

⁸ M. ABRAWOWITZ and I. A. STEGUN, Handbook of Mathematical Functions, National Bureau of Standards, Washington D.C. 1964, Ch. 22.7.15, p. 782.

Moreover, $\sin^2 \alpha$ goes to $\frac{1}{2}$ for large angular momenta $l_1 = L + o(L)$ and $l_2 = L + o(L)$ if the center-of-mass orbital angular momentum L of the cluster becomes large. Hence one is justified to conclude that $\alpha = \pi/4$ and its neighborhood represent energy correlations typical for a cluster and are contained in the basis of energy-correlated channels in the form of large channel quantum numbers n .

However, the mean square deviation

$$\begin{aligned} \Delta &= \frac{\langle (\sin^2 \alpha - \langle \sin^2 \alpha \rangle_{l_1, l_2, n})^2 \rangle_{l_1, l_2, n}}{(n+l_1+\frac{1}{2})(n+l_2+\frac{1}{2})n(n+l_1+l_2+1)(2n+l_1+l_2+3)} \\ &\quad + \frac{(n+l_1-\frac{1}{2})(n+l_2-\frac{1}{2})(n+1)(n+l_1+l_2+2)(2n+l_1+l_2+1)}{(2n+l_1+l_2)^2(2n+l_1+l_2+1)^2(2n+l_1+l_2-1)}, \end{aligned} \quad (30)$$

is $\frac{1}{8} + O(1/n)$ for large n and arbitrary orbital angular momenta l_1, l_2 of the particle, pair, whereas $\Delta = n/[4(n+L)] + o(n^{-1}L^{-1})$ for large center-of-mass orbital angular momentum L of the cluster, i. e. $l_1 = L + o(L)$, $l_2 = L + o(L)$.

The first result, $\Delta = \frac{1}{8}$ for $n \rightarrow \infty$, indicates that there are substantially more correlations included in the basis of energy-correlated channel wave functions than just cluster type correlations while the estimate $\Delta \sim 1/4 L$ for large L says that cluster correlations are the only correlations contained in the correlated channels for large angular momentum $L = l_i + o(L)$.

The interchange of the particles representing the pair corresponds to the transformation $\alpha = \frac{1}{2}\pi - \alpha$ under which the energy-correlation wave function

$$2 \sqrt{\frac{2n+l_1+l_2+2}{\sin 2\alpha}} d_{\frac{1}{2}(l_1+l_2+1), \frac{1}{2}(l_1-l_2)}^{\frac{1}{2}(l_1+l_2+1)+n} (2\alpha) \quad (2\alpha)$$

transforms into

$$2 \sqrt{\frac{2n+l_1+l_2+2}{\sin 2\alpha}} d_{\frac{1}{2}(l_1+l_2+1), \frac{1}{2}(l_1-l_2)}^{\frac{1}{2}(l_1+l_2+1)+n} (2\alpha) (-)^n, \quad (31)$$

indicating the exchange correlations contained in the energy-correlated channel wave function multiplet characterized by fixed channel index $l_1 + l_2 + 2n + \frac{3}{2}$. Each member of the multiplet has the same radial wave function (11). Consequently an antisymmetrized outgoing channel wave function is given by

$$\begin{aligned} &\sqrt{\frac{2(2n+l_1+l_2+2)}{\sin 2\alpha}} \left(d_{\frac{1}{2}(l_1+l_2+1), \frac{1}{2}(l_1-l_2)}^{\frac{1}{2}(l_1+l_2+1)+n} (2\alpha) [Y^{[l_1]}(\hat{r}_1) \times Y^{[l_2]}(\hat{r}_2)]_m^{[l]} \right. \\ &\quad \left. - (-)^{n+l-l_1-l_2} d_{\frac{1}{2}(l_1+l_2+1), \frac{1}{2}(l_1-l_2)}^{\frac{1}{2}(l_1+l_2+1)+n} (2\alpha) [Y^{[l_2]}(\hat{r}_1) \times Y^{[l_1]}(\hat{r}_2)]_m^{[l]} \right). \end{aligned} \quad (32)$$

II. Cluster Channels

Since asymptotically the two-particle cluster (deuteron) wave function $\varphi_d(\varrho)$ is concentrated at $\alpha = \pi/4$ with a range of a few fermi's an expansion of $\varphi_d(\varrho)$ in terms of energy-correlated wave functions would require large quantum numbers n as shown previously. Hence if we restrict the energy-correlated basis of the effective Hilbert space to the few lowest values of n , the cluster channels supplement the correlated channels and are approximately orthogonal to the latter in the asymptotic region, as shown in the next section, i. e. for large r or, equivalently, for large center-of-mass cluster coordinate R .

The channel wave function of the outgoing cluster consists of a product of the center-of-mass wave $\Phi_{LM}(\mathbf{R})$ of orbital angular momentum L, M

$$\begin{aligned} \Phi_{LM}(\mathbf{R}) &= \Phi_L(kR) Y_L^M(\hat{R}) \\ &= \frac{k}{\sqrt{v_c}} [\cos \delta_{j_L}(kR) - \sin \delta_{n_L}(kR)] Y_L^M(\hat{R}) \end{aligned} \quad (33)$$

and the bound cluster wave function $\varphi_v(\boldsymbol{\rho})$ in relative coordinates with respect to its center of mass (see Fig. 2),

$$\begin{aligned} u_{v, LM}(\mathbf{R}, \boldsymbol{\rho}) &= \Phi_{LM}(\mathbf{R}) \varphi_v(\boldsymbol{\rho}) \\ &= \Phi_L(kR) \cdot \varphi_{v, LM}(\boldsymbol{\rho}, \hat{R}). \end{aligned} \quad (34)$$

The spherical Bessel and Neumann functions in (33) of the free cluster have to be replaced by the corresponding regular and irregular Coulomb wave functions for charged clusters.

The cluster wave function $\varphi_v(\varrho)$ represent the various excited states of the cluster. In the case of a deuteron cluster (see Fig. 2)

$$\boldsymbol{\rho} = \mathbf{r}_1 - \mathbf{r}_2. \quad (35)$$

The natural boundary condition

$$\left. \frac{\partial \ln \Phi_L(kR)}{\partial \ln R} \right|_{R=C} \quad (36)$$

for the cluster continuum channel is imposed on the radial center-of-mass wave function $\Phi_L(kR)$.

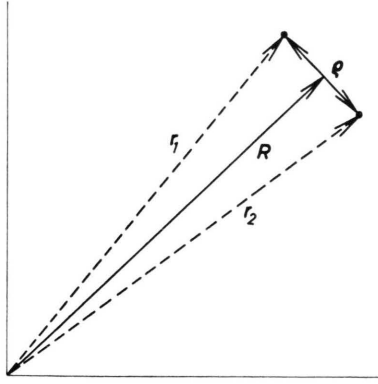


Fig. 2. Relative coordinates with respect to the residual target nucleus of a two-particle cluster channel.

III. Channel Orthogonality

We discuss here the channel orthogonality between the energy-correlated two-particle wave functions Φ_n and the two-particle cluster wave functions, i. e. the deuteron cluster. The extension to multi-particle channels and the Coulomb interaction will be discussed elsewhere.

The bound-state wave function ψ_B of the deuteron cluster including the center-of-mass motion is a solution of the Hamiltonian

$$H = \nabla^2(\mathbf{r}_1) + \nabla^2(\mathbf{r}_2) + k^2 + V_{12} \quad (37)$$

where the interaction V_{12} extends to the asymptotic region while the energy-correlated two-particle wave functions Φ_n represent the solutions of the free Hamiltonian

$$H' = \nabla^2(\mathbf{r}_1) + \nabla^2(\mathbf{r}_2) + k^2. \quad (38)$$

The unbound solutions ψ_F of H are close to the energy-correlated wave functions Φ_n of H' because of the short-ranged potential V_{12} .

As we intend to use the Φ_n instead of ψ_F as basis of the Hilbert space we have to estimate channel orthogonality which we know holds approximately in the asymptotic region.

First, let us write the center-of-mass coordinate of the deuteron

$$\mathbf{R} = \frac{1}{2} (\mathbf{r}_1 + \mathbf{r}_2)$$

and the relative cluster coordinate

$$\boldsymbol{\rho} = \mathbf{r}_1 - \mathbf{r}_2$$

in terms of the asymptotic coordinates $\alpha, r, \hat{r}_1, \hat{r}_2$,

$$\varrho = r[1 - \sin 2\alpha \hat{r}_1 \cdot \hat{r}_2]^{\frac{1}{2}} \quad (39a)$$

$$\text{and} \quad R = \frac{1}{2} r[1 + \sin 2\alpha \hat{r}_1 \cdot \hat{r}_2]^{\frac{1}{2}}. \quad (39b)$$

Since the bound-state wave function $\varphi_d(\varrho)$ of the deuteron decreases exponentially beyond the deuteron volume characterized by the radius d , say, we consider only this region

$$\varrho \leq d, \quad \text{i. e.} \quad \alpha = \frac{1}{4}\pi + O(1/R),$$

so that up to second order terms in $\Delta\alpha = \frac{1}{4}\pi - \alpha$ and $\cos 2\vartheta = \hat{r}_1 \cdot \hat{r}_2 = 1 - 2\vartheta^2$ one obtains upon expanding

$$\varrho = r[2((\Delta\alpha)^2 + \vartheta^2)]^{\frac{1}{2}} \quad (40a)$$

$$\text{and} \quad R = (r/\sqrt{2})[1 - \frac{1}{2}((\Delta\alpha)^2 + \vartheta^2)], \quad (40b)$$

where consequently

$$\Delta\alpha = (1/R) f(\varrho) \quad \text{and} \quad \vartheta = (1/R) g(\varrho).$$

$$\Delta\alpha = (1/R) f(\varrho) \quad \text{and} \quad \vartheta = (1/R) g(\varrho).$$

The complete asymptotic channel wave function consists of a radial and a hypersurface component, depending on the (bounded) variables $\alpha, \hat{r}_1, \hat{r}_2$, and the latter is used to project out the radial part from which the phase shifts are extracted. We are, therefore, only interested in the overlap of the cluster and correlated pair channel wave functions over the channel hypersurface.

Substituting Eq. (40b) in the form

$$R = r/\sqrt{2} \quad \text{and} \quad dR = dr/\sqrt{2} \quad (41)$$

into the complete channel volume element in relative and center-of-mass coordinates,

$$R^2 dR d\varrho^2 d\varrho d\hat{\varrho} = r^5 dr \frac{1}{4} \sin^2 2\alpha d\alpha d\hat{r}_1 d\hat{r}_2 \quad (42)$$

the channel hypersurface volume element

$$\frac{1}{4} \sin^2 2\alpha d\alpha d\hat{r}_1 d\hat{r}_2 = (1/8 R^3) d\hat{R} d\varrho^2 d\varrho d\hat{\varrho} \quad (43)$$

results.

Thus the hypersurface channel coordinates for the cluster are \hat{R} and $\boldsymbol{\rho}$. If we use the channel surface volume in pair coordinates in the form

$$dS = r^5 \cdot \frac{1}{4} \sin^2 2\alpha d\alpha d\hat{r}_1 d\hat{r}_2 \quad (44)$$

so that the channel volume element

$$d\tau = dr dS,$$

then the normalized surface channel wave function [see Eq. (24)] is

$$\tilde{\psi}_{n l_1 l_2} = r^{-5/2} 2 \left[\frac{2n+l_1+l_2+2}{\sin 2\alpha} \right]^{1/2} d_{\frac{1}{2}(l_1+l_2+1), \frac{1}{2}(l_1-l_2)}^{1/2(l_1+l_2+1)+n} (2\alpha) \cdot [Y^{[l_1]}(\hat{r}_1) \times Y^{[l_2]}(\hat{r}_2)]_m^{[L]} \quad (45)$$

with $\int |\tilde{\psi}_{n l_1 l_2}|^2 dS = 1$.

The radial outgoing component O_c behaves as

$$O_c = \sqrt{\pi k r / (2v)} H_{2n+l_1+l_2+2}^{(1)}(kr) \sim (1/v) \exp\{i[kr - \frac{1}{2}\pi(2n+l_1+l_2 + \frac{5}{2})]\} \quad (46)$$

so that the complete channel wave function ψ_p is (asymptotically) normalized to unit pair flux,

$$\int \left(\psi_p^* \frac{\hbar}{2im} \frac{\partial}{\partial r} \psi_p - \psi_p \frac{\hbar}{2im} \frac{\partial}{\partial r} \psi_p^* \right) dS \sim \frac{\hbar k}{mv} = 1.$$

At the location of the cluster the center-of-mass spherical wave Φ_{LM} of the two-particle cluster channel wave function, splits off the radial part, using $R = r/\sqrt{2}$, which must be similarly normalized to unit pair flux.

The normalized surface channel wave function is

$$\tilde{\psi}_{d, LM} = (2^{1/4}/R) Y_L^M(\hat{R}) \varphi_d(\varrho) \quad (47)$$

and the channel surface volume element

$$dS = (1/\sqrt{2}) R^2 dR \varrho^2 d\varrho \quad (48)$$

so that $\int |\tilde{\psi}_{d, LM}|^2 dS = 1$

holds.

$\varphi_d(\varrho)$ denotes the deuteron ground-state wave function. For more general clusters one has to couple the angular momentum of the cluster and of the center of mass to a total angular momentum. The radial outgoing component O_d of the cluster channel wave function asymptotically behaves as

$$O_d = (kR/\sqrt{v_c}) h_L^{(1)}(kR) \sim (1/\sqrt{v_c}) \exp\{i(kR - \frac{1}{2}\pi(L+1))\} \quad (49)$$

where v_c is the center-of-mass cluster velocity so that the complete cluster channel wave function is (asymptotically) normalized to unit two-particle flux

$$\int \left(\psi_{d, LM}^* \frac{\hbar}{2im_c} \frac{\partial}{\partial R} \psi_{d, LM} - \psi_{d, LM} \frac{\hbar}{2im_c} \frac{\partial}{\partial R} \psi_{d, LM}^* \right) dS \sim \frac{\hbar k}{m_c v_c} = 1.$$

The deuteron wave function φ_d restricts the range of integration in the orthogonality overlap integral to the deuteron volume so that because of

$$\hat{r}_1 = \hat{r}_2 = \hat{R}, [Y^{[l_1]}(\hat{r}_1) \times Y^{[l_2]}(\hat{r}_2)]_M^{[L]} = \left(\frac{(2l_1+1)(2l_2+1)}{4\pi} \right)^{1/2} (-)^{l_1-l_2} \begin{pmatrix} l_1 & l_2 & L \\ 0 & 0 & 0 \end{pmatrix} Y_L^M(\hat{R}). \quad (50)$$

We are thus led to estimate the overlap integral

$$O_{n l_1 l_2 LM} = \int \tilde{\psi}_{n l_1 l_2} \tilde{\psi}_{d, LM}^* dS = \int r^5 \frac{\sin^2 2\alpha}{4} d\alpha d\hat{r}_1 d\hat{r}_2 \frac{2^{3/4}}{r} \varphi_d(|\mathbf{r}_1 - \mathbf{r}_2|) Y_L^M(\hat{R}) \frac{2}{r^{5/2}} \left(\frac{l_1+l_2+2+2n}{\sin 2\alpha} \right)^{1/2} \times d_{\frac{1}{2}(l_1+l_2+1), \frac{1}{2}(l_1-l_2)}^{1/2(l_1+l_2+1)+n} (2\alpha) [Y^{[l_1]}(\hat{r}_1) \times Y^{[l_2]}(\hat{r}_2)]_M^{[L]} \quad (51)$$

which by inserting (48) and (50) transforms into

$$O_{n l_1 l_2 LM} \frac{1}{\sqrt{2} R^{5/2}} \left[\frac{(l_1+l_2+2+2n)(2l_1+1)(2l_2+1)}{4\pi} \right]^{1/2} (-)^{l_1-l_2} \begin{pmatrix} l_1 & l_2 & L \\ 0 & 0 & 0 \end{pmatrix} \cdot \int d\hat{R} Y_L^M(\hat{R}) Y_L^M(\hat{R}) \cdot \int \frac{1}{\sqrt{\sin 2\alpha}} d_{\frac{1}{2}(l_1+l_2+1), \frac{1}{2}(l_1-l_2)}^{1/2(l_1+l_2+1)+n} (2\alpha) \cdot \varphi_d(\varrho) d^3\varrho. \quad (52)$$

Since $\sin 2\alpha = 1 + O(1/R)$ and consequently

$$d_{\frac{1}{2}(l_1+l_2+1), \frac{1}{2}(l_1-l_2)}^{1/2(l_1+l_2+1)+n} (2\alpha) = d_{\frac{1}{2}(l_1+l_2+1), \frac{1}{2}(l_1-l_2)}^{1/2(l_1+l_2+1)+n} (\pi/2) \quad (53)$$

all over the deuteron volume, we obtain

$$O_{n l_1 l_2 LM} = \frac{(-1)^{l_1-l_2}}{R^{5/2} \sqrt{2}} \left(\frac{(l_1+l_2+2n+2)(2l_1+1)(2l_2+1)}{4\pi} \right)^{1/2} \begin{pmatrix} l_1 & l_2 & L \\ 0 & 0 & 0 \end{pmatrix} d_{\frac{1}{2}(l_1+l_2+1), \frac{1}{2}(l_1-l_2)}^{1/2(l_1+l_2+1)+n} (\pi/2) \cdot \int \varphi_d(\varrho) d^3\varrho. \quad (54)$$

The normalization of the deuteron wave function $\varphi_d(\varrho)$ implies that

$$|\int \varphi_d(\varrho) d^3\varrho| \leq (\int |\varphi_d(\varrho)|^2 d^3\varrho)^{1/2} (\int d^3\varrho)^{1/2} \leq (V_d)^{1/2} \quad (55)$$

so that the final estimate for the channel orthogonality overlap reads

$$|O_{n l_1 l_2 LM}| \leq \sqrt{\frac{V_d}{R^3}} \frac{1}{\sqrt{2}} \left[\frac{(l_1+l_2+2n+2)(2l_1+1)(2l_2+1)}{4\pi} \right]^{1/2} \cdot \left| \begin{pmatrix} l_1 & l_2 & L \\ 0 & 0 & 0 \end{pmatrix} d_{\frac{1}{2}(l_1+l_2+1), \frac{1}{2}(l_1-l_2)}^{1/2(l_1+l_2+1)+n} (\pi/2) \right|. \quad (56)$$

From Eq. (56) it is clear that, for channel orthogonality to hold, the two-particle matching radius $R = c/\sqrt{2}$ must be chosen large enough so that the ratio of cluster volume V_d versus interior interaction region, i. e. the channel overlap probability becomes as small as required by the numerical accuracy.

Of course, the estimate for $O_{n l_1 l_2 LM}$ in Eq. (56) is meaningful only for small quantum numbers l_1, l_2, L, n compared to the ratio R^3/V_d .

Since no special properties of the cluster wave function were used we notice that the estimate in Eq. (56) with minor changes due to coupling coefficients applies also to the more general case of two simultaneously outgoing and energy-correlated clusters and the bound compound system consisting of these two clusters in any excited state.

IV. Schematic Solution of the Hamiltonian

1. The S-Matrix

In the eigenchannel representation the S-matrix is defined to be diagonal, i. e.

$$S V^{(\beta)} = \exp\{2 i \delta^{(\beta)}\} V^{(\beta)} \quad (57)$$

so that an arbitrary element $S_{CC'}$ of the scattering matrix is given by

$$S_{CC'} = \sum_{\beta} V_C^{(\beta)} \exp\{2 i \delta^{(\beta)}\} V_{C'}^{(\beta)*}. \quad (58)$$

The channel labels C, C' stand for the single-particle and two-particle continuum channel quantum numbers (N_ν, j_ν, \dots) and (n, l_1, l_2, l, \dots) , respectively. Consequently the eigenchannel index β in Eq. (58) runs over a denumerable set. But at a given primary energy only a finite number of channels are open in practice so that actually only a finite number of eigenchannels β contribute to each S-matrix element $S_{CC'}$ connecting two experimental channels C, C'. This is correct as long as one restricts the correlated two-particle channels to the lowest quantum numbers $n=0, 1, 2, \dots$ of Eq. (24). Thus, in practice, we have at this point an important approximation which replaces the correlated two- (and more) particle channels of high channel index by cluster channels. As is discussed in Section I the most important energy-correlated channels involved in a particular reaction can be read off the experimental cross section for particle pairs as a function of the energy partition angle α yielding a lower bound for the

cut-off channel index quantum number n_{\max} which otherwise is arbitrary and depends on the numerical accuracy desired. The two-particle matching radius is chosen subsequently depending on the bounds imposed by the required numerical accuracy on the channel orthogonality overlap integrals. According to the conventional definition of the S-matrix in terms of the incoming and outgoing channel amplitudes A_C, B_C , one has

$$B_C = - \sum_{C'} S_{C'C} A_{C'}. \quad (59)$$

Because of the unitarity of the S-matrix all eigenphases $\delta^{(\beta)}$ are real. It is obvious from the definition of the eigenchannels in Eq. (57) that in general eigenchannels are different from experimental channels.

The eigenchannel wave functions represent superpositions of standing waves in each eigenchannel β because asymptotically, assuming for simplicity neutral particles, one has

$$\begin{aligned} \psi^{(\beta)} &= \sum_C (V_C^{(\beta)} I_C - \exp\{2 i \delta^{(\beta)}\} V_C^{(\beta)} O_C) \tilde{\psi}_C \quad (60) \\ &\sim \sum_{(k_C r_C \rightarrow \infty)} V_C^{(\beta)} \exp\{i \delta^{(\beta)}\} [\exp\{-i(k_C r_C + \delta^{(\beta)} - l_C \pi/2)\} - \exp\{i(k_C r_C + \delta^{(\beta)} - l_C \pi/2)\}] \tilde{\psi}_C. \end{aligned}$$

As is usual in reaction theory, I_C and O_C denote the radial parts of the incoming and outgoing particles in the physical (experimental) channel C, i. e.

$$(k R/2 \sqrt{v_C}) [e^{i\delta} h_L^{(1)}(k R) + e^{-i\delta} h_L^{(2)}(k R)]$$

for a cluster channel and

$$\sqrt{k r/v} [e^{i\delta} H_{l_1+l_2+2n+2}^{(1)}(k r) + e^{-i\delta} H_{l_1+l_2+2n+2}^{(2)}(k r)] \quad (61)$$

for an energy-correlated channel, whereas $\tilde{\psi}_C$ denotes the channel wave function.

The same notation applies to the eigenchannels β . The channel amplitudes $V_C^{(\beta)}$ in Eq. (57) can be obtained from the nuclear wave function by projection using the asymptotically orthogonal channel wave functions $\tilde{\psi}_C$. Once the complete nuclear eigenchannel wave function $\psi^{(\beta)}$ is known in the inner interaction region and the eigenphase shifts $\delta^{(\beta)}$ are calculated using the iteration procedure typical for the eigenchannel method³, the total S-matrix is known for the particular energy. In the asymptotic region each experimental, i. e. physically realistic wave function is a linear superposition of eigenchannel wave functions. In other words, the eigenchannel amplitudes $V_C^{(\beta)}$ represent the column vectors of an

orthogonal matrix transforming the asymptotic experimental channel wave functions into the eigenchannel wave functions which diagonalize the scattering matrix and represent coupled channel wave functions. Since each eigenchannel depends on only one eigenphase which can be determined by variation the eigenchannel method easily generalizes to nuclear reactions above the two-particle emission threshold.

2. Solution of the Hamiltonian

The first step toward the solution of the nuclear Hamiltonian inside the internal interaction region consists in constructing a complete basis of antisymmetrized states. Since above the two-particle threshold in general a large number of one- and two-particle channels is open we intend to restrict considerably the space of configurations involved. The dimension of this minimal effective Hilbert space in which the shell model Hamiltonian is diagonalized becomes a function of the energy of the particular reaction.

The main objective of the eigenchannel method is to deal rigorously and as simply as one possibly can with the particle continua in nuclear reactions. The method also stays close to the usual bound state shell model calculation. Its main feature is to operate with a unitary transformation matrix on the asymptotic channel wave functions so that firstly the S -matrix becomes diagonal and secondly the transformed new channel wave functions (coupled physical channel wave function) depend on only one phase shift δ each. One has to solve the equation

$$E(\delta) = E \quad (62)$$

for the phase shift δ . The energy eigenvalues $E(\delta)$ are the solutions of the Hamiltonian inside the internal interaction region. Each eigenphase $\delta^{(\beta)}$ is determined by variation so that even in the case of several coupled channels only one $\delta^{(\beta)}$ is calculated at a time. This procedure simplifies considerably the numerical determination of the phase shifts $\delta^{(\beta)}$, for which one has, however, to pay in that all energy matrix elements $H_{ik}(\delta^{(\beta)})$ explicitly depend on the phase shift $\delta^{(\beta)}$ involved.

A second characteristic of virtually all shell model calculations is the restriction of the complete Hilbert space to a minimal space of configurations in which the Hamiltonian is diagonalized. Far below the 2-

particle emission threshold one needs consider approximately, only $1p-1h$ configurations of the compound A -particle system. Above the 2-particle threshold the $(1p-1h)$ - and $(2p-2h)$ -Hilbert space has, in practice, also to be restricted. Consequently the completeness is explicitly violated. One can, however, approximately account for the neglect of some not essential degrees of freedom by using an effective interaction whose parameters have to be adjusted to the experiment. They can, for example, be fitted on one particular reaction. All other matrix elements of the S -matrix are then parameter-free predictable. The dimensions of such a minimal extension of the shell model Hilbert space obviously becomes an energy-dependent parameter. This drawback is a general feature of any attempt so far to include the effects of the particle continua. On the other hand, the dependence of the scattering cross sections on this parameter serves as a criterion to determine the size of the effective Hilbert space involved at a given reaction energy. One can test the sensitivity of the results on the cut-off of the Hilbert space explicitly and choose, if necessary, a larger Hilbert space. Of course, the actual size of the minimal Hilbert space can be determined only numerically.

There are indications that the effective Hilbert space is of reasonably small dimension: The coupled channel and eigenchannel methods which attempt to treat rigorously the one-particle continuum do not seem to exhibit qualitatively new features as compared to the ordinary shell model calculations. The reason may be that only a relatively small number ($\lesssim 20$) of states of the one-particle continua essentially contribute to each reaction channel.

3. Detailed Construction of a Minimal Basis

One needs a complete set of states in the interior region in order to diagonalize the nuclear Hamiltonian. There are three kinds of states: 1) one-particle states where only one particle is in the continuum and may escape which are denoted by $u_\nu(\mathbf{r}_\infty)$ and defined in the interval $0 \leq r_\infty \leq b$ (see Fig. 3). 2) The correlated two-particle states where two particles are in the continuum and both particles may escape. They are denoted by $\Phi_n(r, \alpha)$ and defined in the space $0 \leq r \leq c$ (see Fig. 3). 3) The cluster wave functions $\chi_m(\mathbf{R}, \mathbf{p})$ which are defined in the space $0 \leq R \leq c/\sqrt{2}$. The factor $1/\sqrt{2}$ is convenient

here because it follows from (39 b) that asymptotically $R = r/\sqrt{2}$ (see Fig. 3).

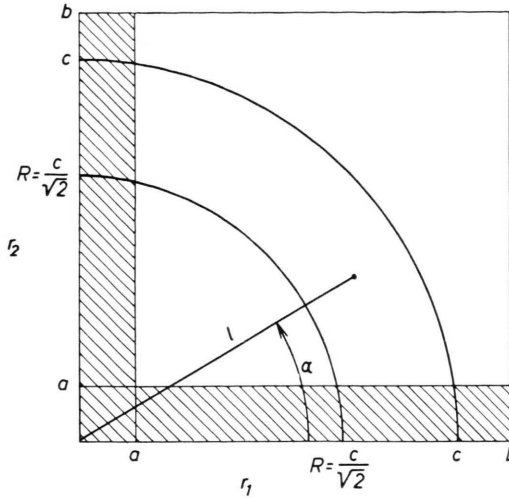


Fig. 3. The one-particle channels are matched to the asymptotic region by a boundary condition at $r_1, r_2 = b$, the two-particle energy-correlated channels at $r = c$ and the cluster (deuteron) channels at $R = c/\sqrt{2}$. The internal interaction region is defined by $r \leq c$. Channel orthogonality is violated in the cross-hatched region because for $r_1 < c$ or $r_2 < c$ the wave function is not of the asymptotic form.

The single particle wave functions

$$u_v(\mathbf{r}_\kappa) = R_L(r_\kappa) Y_l^m(\hat{r}_\kappa)$$

are solutions of a Saxon-Woods shell model Hamiltonian satisfying the natural boundary condition.

$$\left. \frac{\partial \ln R_L(r_\kappa)}{\partial \ln r_\kappa} \right|_{r_\kappa=b} = \frac{\partial}{\partial \ln(r_\kappa)} \cdot \ln [\cos \delta j_L(k r_\kappa) - \sin \delta n_L(k r_\kappa)] \Big|_{r_\kappa=b} \quad (63)$$

They are, consequently, normalized over the volume $r_\kappa \leq b$.

The two-particle correlated wave function is

$$\begin{aligned} \Phi_{\lambda, N}(r, \alpha) = N \frac{1}{r^2} J_{l_1+l_2+2n+2}(k_\lambda r) 2 \left(\frac{l_1+l_2+2n+2}{\sin 2\alpha} \right)^{\frac{1}{2}} \\ \cdot d_{\frac{1}{2}(l_1+l_2+1), \frac{1}{2}(l_1-l_2)}^{\frac{1}{2}(l_1+l_2+1)+n} (2\alpha) \cdot [Y^{[l_1]}(\hat{r}_1) \times Y^{[l_2]}(\hat{r}_2)]_m^{[l]} \end{aligned} \quad (64)$$

whose radial wave function $J_{l_1+l_2+2n+2}(k_\lambda r)$ satisfies the boundary condition

$$\begin{aligned} \left. \frac{\partial \ln J_{l_1+l_2+2n+2}(k_\lambda r)}{\partial \ln r} \right|_{r=c} \\ = \frac{\partial}{\partial \ln r} \ln (\cos \delta J_{l_1+l_2+2n+2}(k_\lambda r) - \sin \delta N_{l_1+l_2+2n+2}(k_\lambda r)) \Big|_{r=c} \end{aligned} \quad (65)$$

from which the discrete set of energies k_λ results. These wave functions (64) are normalized within $r \leq c$.

The free cluster wave functions

$$\chi_{a, M}(\mathbf{R}, \boldsymbol{\rho}) = N' F_L(k_a R) \varphi(\boldsymbol{\rho}) Y_L^M(\hat{R}) \quad (66)$$

are normalized in the inside region within $R \leq c/\sqrt{2}$. F_L and G_L denote the regular and irregular Coulomb wave functions, respectively. The radial functions are subject to the boundary condition

$$\begin{aligned} \left. \frac{\partial \ln F_L(k_a R)}{\partial \ln R} \right|_{R=c/\sqrt{2}} \\ = \frac{\partial \ln (\cos \delta F_L(k_a R) + \sin \delta G_L(k_a R))}{\partial \ln R} \Big|_{R=c/\sqrt{2}}. \end{aligned} \quad (67)$$

It should be noticed that the basis functions of both, the correlated two-particle functions (64) and the cluster functions (63) are solutions of the free equations of motion (without 1-body potential) in the inside region. Thus the full Hamiltonian has to be diagonalized later.

We have thus obtained three sets of functions u_v , $\Phi_{\lambda, N}$ and $\chi_{a, M}$ which are defined in the three different spaces shown in Fig. 3. As has been discussed in ref. ², the functions $\Phi_{\lambda, N}$ and $\chi_{a, M}$ are now expanded in terms of the two-particle functions $u_v(\mathbf{r}_1) u_\mu(\mathbf{r}_2)$ which are defined in the space $r_1, r_2 \leq b$ (see Fig. 3). Furthermore, the solutions $\Phi_{\lambda, N}$ and $\chi_{a, M}$ are extended beyond their original space of definition into the full space $r_1, r_2 \leq b$ and orthonormalized there. This leads to the new set of one-particle, two-particle and cluster functions u_v , $\bar{\Phi}_{\lambda, N}$, $\bar{\chi}_{a, M}$ defined in $r_1, r_2 \leq b$. The redundant states are eliminated as discussed in reference ², and the full Hamiltonian is diagonalized in this basis.