Eigenchannel Theory of Nuclear Reactions*

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A method is proposed by which the eigenstates and the eigenvalues of the S matrix, i.e., the eigenchannels, can be directly computed from the nuclear problem, for example, from the shell model. The calculation of all cross sections, viz., partial and total cross sections, is then exceedingly simple. The characteristics of the eigenchannels are described and the relation with other reaction theories is briefly discussed.

I. INTRODUCTION

IN a recent paper[1] we have developed a formalism for the treatment of narrow resonances by shell-model methods. In this paper we shall generalize the treatment to the case of arbitrary continuum states. A central role here again is played by the natural boundary conditions. However, we abandon the previously used R-matrix theory and use, instead, a representation in which the S matrix is diagonal. In this representation all formal relations are very simple and transparent. We shall call the eigenstates of the S matrix the "eigenchannels" and the phase shifts associated with the eigenvalues of the S matrix the "eigenphases." As will be seen below the eigenchannels and the eigenphases can be obtained directly from the shell model. To this end, the configuration space is separated into an inside and an outside region. The nuclear problem is solved in the inside region by using properly defined natural boundary conditions for the wave function at the matching radius, $r=a$, which separates the inside and the outside regions; the obtained solutions are already without further transformations the eigenchannel solutions.

The previously treated case of a narrow resonance[1] corresponds to the situation in which the reaction is dominated by a single compound state, and which can be described by a single-level Breit-Wigner formula. In the eigenchannel language this corresponds to the domination of the reaction by a single eigenchannel, which has at the resonance energy an eigenphase of $\pi/2$. Then all the other channels can be relegated to the "background."

In general *all* eigenchannels contribute comparably to the reaction amplitude. It is thus necessary to find all eigenchannels and all eigenphases. Once this has been done one actually has obtained the complete solution of the problem. This can be seen formally very simply. Writing the eigenvalue equation as

$$SV^{(\alpha)}=\epsilon_\alpha V^{(\alpha)}, \tag{1}$$

then the eigenvalues can be written in the form

$$\epsilon_\alpha=e^{2i\delta_\alpha}, \tag{2}$$

where, because of the unitarity of the S matrix, the eigenphases δ_α are real. Combining the column vectors $V^{(\alpha)}$ into a "solution matrix" W and constructing with the eigenvalues $e^{2i\delta_\alpha}$ the eigenvalue matrix ϵ which is a diagonal matrix whose diagonal elements are the eigenvalues ϵ_α, we have the well-known representation[2] of the S matrix

$$S=W\epsilon W^{-1}, \tag{3}$$

which, then, is the complete formal solution of the problem.

Evidently, the formal aspects of the reaction theory are so trivial in the present treatment that it even may not deserve the name "reaction theory." However, for exactly the same reason we believe that it is eminently suited as a method for the computation of reaction cross sections. Actual numerical calculations using this method are underway at this time. They will be reported on in a separate publication.

There exist several procedures in the literature for treating the problem of this paper.[3-7] In fact, the simplest cases, e.g., O^{16} in the one-particle–one-hole approximation, can be treated by every method. Which of the methods is easier to apply, and which of the methods is easier to generalize to more complicated systems and to higher approximations, will have to be proven out by practical experience.

In the present paper we still limit ourselves to the energy region below the two-particle threshold, i.e., all considered channels are assumed to have only a single incoming or outgoing particle. Also, the center-of-mass problem has been left unresolved. However, this is a separate problem, and it would disappear simply by using such wave functions in which the spurious components have been eliminated by means of some arbitrary, although as yet unknown, prescription. Without this refinement, the results will contain uncertainties of the order $1/A$.

In Sec. II we give the precise definition of the eigenchannels and discuss their physical meaning; we also

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describe some special cases. Some formal relations are discussed in Sec. III. The procedure for computing the S matrix is given in Sec. IV. Many details of this procedure can be taken over completely from Ref. 1. In Sec. V we show in which way resonating and nonresonating processes appear in the eigenchannel method and discuss the relations of this method with the R-matrix formalism.

II. THE EIGENCHANNELS

In this section we give the precise definitions of the eigenchannels and discuss their physical meaning. The S matrix is defined, as usually, by the asymptotic form of the wave function, i.e., by the wave function at such distances where the short-range nuclear forces have a negligible magnitude. There then holds

$$\Psi=\sum_c [A_c I_c+B_c 0_c]\tilde{\psi}_c. \tag{4}$$

Here I_c and 0_c are the radial parts of the incoming and outgoing particle in the channel c, $\tilde{\psi}_c$ is the wave function of the $(A-1)$ system together with the angular parts of the projectile particle, and the summation is over all open channels. To distinguish these channels c from the eigenchannels of the S matrix, we shall call them the "experimental channels." The S matrix then is defined by

$$B_c=-\sum_{c'} S_{cc'}A_{c'}. \tag{5}$$

Considering (1) and (2), and assuming neutral particles, it then holds that for an eigenchannel

$$\begin{aligned}\Psi^{(\alpha)}&=\sum_c [V_c^{(\alpha)}I_c-e^{2i\delta_\alpha}V_c^{(\alpha)}0_c]\tilde{\psi}_c\\&=\sum_c V_c^{(\alpha)}e^{i\delta_\alpha}[e^{-i\delta_\alpha}I_c-e^{i\delta_\alpha}0_c]\tilde{\psi}_c\\&\rightarrow\sum_c V_c^{(\alpha)}e^{i\delta_\alpha}[^{-i(k_c r_c+\delta_\alpha-l_c\pi/2)}\\&\qquad -e^{i(k_c r_c+\delta_\alpha-l_c\pi/2)}]\tilde{\psi}_c\\&=-2ie^{i\delta_\alpha}\sum_c V_c^{(\alpha)}\sin(k_c r_c+\delta_\alpha-l_c\pi/2)\tilde{\psi}_c.\end{aligned} \tag{6}$$

The eigenchannel thus corresponds to standing waves in all open experimental channels with a common phase shift, the eigenphase δ_α. This is true also for channels in which the outgoing particle is charged.

We now turn to the discussion of (3), i.e., to the representation of the S matrix in terms of the eigenchannels and eigenphases. The solution matrix W which has the elements

$$W_{ik}\equiv V_i^{(k)} \tag{7}$$

can always be inverted since the solutions $V^{(\alpha)}$ form a complete set. In particular, there are as many eigenchannels as there are open experimental channels at the considered energy, say N. The vectors $V^{(\alpha)}$ are orthogonal as long as the eigenphases are nondegenerate. Otherwise they can be orthogonalized. Furthermore, they can be normalized. From now on we shall assume that the ortho-normalization has indeed been carried out. Then

$$W^{-1}=\tilde{W}^*, \tag{8}$$

and together with the definition of the eigenvalue matrix elements

$$\epsilon_{ik}=\epsilon_i\delta_{ik}, \tag{9}$$

Eq. (3) becomes

$$S_{cc'}=\sum_\alpha V_c^{(\alpha)}e^{2i\delta_\alpha}V_{c'}^{(\alpha)*}. \tag{10}$$

Equation (10) shows that in the end no matrix inversions are necessary if the complete set of eigenchannels has been obtained. It remains to be shown that in fact it is possible to obtain such solutions. Before turning to that qestion we discuss some special cases of the S matrix.

In potential scattering the different experimental channels do not mix and the S matrix is thus diagonal in the experimental channel representation. Here the experimental channels are already the eigenchannels. The different eigenphases have no relation to each other.

Somewhat more tricky is the case of degeneracy of eigenphases. Let us consider the case where a certain number, say n, of the eigenphases are equal. Then, writing M for the inverse of the W matrix (8), i.e., putting $M=W^{-1}$, and writing $\mathbf{1}_n$ for the n-dimensional unit matrix, we have

$$S=\begin{pmatrix}W_{\alpha\alpha} & W_{\alpha\beta}\\ W_{\beta\alpha} & W_{\beta\beta}\end{pmatrix}\begin{pmatrix}\mathbf{1}_n\Delta & 0\\ 0 & \Gamma_\beta\end{pmatrix}\begin{pmatrix}M_{\alpha\alpha} & M_{\alpha\beta}\\ M_{\beta\alpha} & M_{\beta\beta}\end{pmatrix}, \tag{11}$$

which is (3) expanded such that the degenerate states are explicitly separated from the nondegenerate states. Furthermore, we have written $\Delta=e^{2i\delta}$ for the degenerate eigenvalues and Γ_β for the diagonal eigenvalue matrix of the other eigenchannels. Note that the first subscript of W and the second subscript of M designate the experimental channels; the eigenchannels are associated with the second subscript in W and the first in M.

Equation (11) can be rewritten as

$$\begin{aligned}S&=\mathbf{1}_N\Delta\\&+\begin{pmatrix}W_{\alpha\beta}[\Gamma_\beta-\mathbf{1}_m\Delta]M_{\beta\alpha} & W_{\alpha\beta}[\Gamma_\beta-\mathbf{1}_m\Delta]M_{\beta\beta}\\ W_{\beta\beta}(\Gamma_\beta-\mathbf{1}_m\Delta]M_{\beta\alpha} & W_{\beta\beta}[\Gamma_\beta-\mathbf{1}_m\Delta]M_{\beta\beta}\end{pmatrix}.\end{aligned} \tag{12}$$

Here $m=N-n$ is the number of nondegenerate eigenchannels.

The S matrix thus splits into two parts, a diagonal part and a nondiagonal part. The latter depends only on the nondegenerate eigenvectors. This can be seen more clearly by writing out explicitly the matrices making up (12), for example,

$$\begin{aligned}&(W_{\alpha\beta}[\Gamma_\beta-\mathbf{1}_m\Delta]M_{\beta\beta})_{cc'}\\&\qquad=\sum_\beta V_c^{(\beta)}[e^{2i\delta_\beta}-e^{2i\delta}]V_{c'}^{(\beta)*}.\end{aligned} \tag{13}$$

We thus see that a degeneracy leads in a certain sense to a "decoupling" of the channels, which is a manifestation of the freedom associated with the arbitrariness of the choice of the degenerate eigenvectors. Any linear combination of degenerate eigenvectors is itself

an eigenvector. Complete degeneracy leads to a complete decoupling of the channels. However, as long as even one eigenvalue is nondegenerate, a well-defined, in general finite, inelastic-scattering cross section does exist, in general connecting all channels. Since the eigenphases are functions of the energy, two eigenphases may coincide at some energy. If at that energy only very few channels are open then, under favorable conditions, the resulting "decoupling" could be observed, e.g., in the branching ratios.

III. DECOMPOSITION OF THE S MATRIX

In this section we discuss a formal decomposition of the S matrix in terms of "S matrices" defined within one eigenchannel.

In the asymptotic region, the most general wave function is given in terms of the eigenchannel wave functions (6) as

$$\Psi=\sum_\alpha q^{(\alpha)}\Psi^{(\alpha)} =\sum_\alpha q^{(\alpha)}\sum_c[V_c{}^{(\alpha)}\mathcal{J}_c+\bar{V}_c{}^{(\alpha)}\mathcal{O}_c]. \tag{14}$$

We have here introduced the abbreviations

$$\bar{V}_c{}^{(\alpha)}=-e^{-2i\delta_\alpha}V_c{}^{(\alpha)*},$$
$$\mathcal{J}_c=I_c\bar{\psi}_c;\quad \mathcal{O}_c=O_c\bar{\psi}_c. \tag{15}$$

A particular wave function describes the situation in which an incoming wave exists in only one channel, say c, and outgoing waves exist in all channels. This is the situation in which the S matrix can be defined in the most immediate manner. We denote the eigenchannel amplitudes describing this situation by $q_c{}^{(\alpha)}$. Thus we have

$$\sum_\alpha q_c{}^{(\alpha)}V_{c'}{}^{(\alpha)}=\delta_{cc'}. \tag{16}$$

Recalling the definition of the solution matrix W in (7) we find immediately

$$q_c{}^{(\alpha)}=-M_{\alpha c}. \tag{17}$$

Inserting (17) in (14) we obtain indeed

$$\Psi=\mathcal{J}_c-\sum_{c'}\sum_\alpha W_{c'\alpha}\epsilon_\alpha M_{\alpha c}\mathcal{O}_{c'}, \tag{18}$$

i.e., the defining equation of the S matrix.

We now define the "eigenchannel S matrix" by the equation

$$\bar{V}_{c'}{}^{(\alpha)}=-\sum_c U_{c'c}{}^{(\alpha)}V_c{}^{(\alpha)}. \tag{19}$$

Inserting (19) into (14) we find

$$S_{c'c}=\sum_{\alpha c''}U_{c'c}{}^{(\alpha)}W_{c''\alpha}M_{\alpha c}, \tag{20}$$

which shows that a possible solution of (10) is

$$U_{c'c}{}^{(\alpha)}=\epsilon_\alpha\delta_{c'c}, \tag{21}$$

which is immediately obvious. However, (19) has an infinite set of solutions[8] which is evident by counting the number of unknowns and the number of equations.

[8] C. Mahaux and H. A. Weidenmüller, Ann. Phys. (N. Y.) 32, 259 (1965).

Another solution is obtained when making the ansatz

$$U_{c'c}{}^{(\alpha)}=\epsilon_\alpha\tau_c{}^{(\alpha)}\tau_{c'}{}^{(\alpha)}, \tag{22}$$

which when inserted in (19) shows that

$$\tau_c{}^{(\alpha)}=V_c{}^{(\alpha)}f^{(\alpha)}, \tag{23}$$

with the normalization constant

$$1/f^{(\alpha)2}=\sum_c(V_c{}^{(\alpha)})^2, \tag{24}$$

which is not necessarily real. Inserting (22) into (20) we again obtain (10). We see that even though (19) has no unique solution, such a definition still may be of use since one always can construct the S matrix using the U matrices if one has a calculational procedure which gives a particular set of solutions.

IV. COMPUTATION OF THE EIGENCHANNELS AND EIGENPHASES

The amplitudes $V_c{}^{(\alpha)}$ and the eigenphases δ_α have to be supplied for each energy of the compound system by the solution of the nuclear Schrödinger equation. This can be done by a method similar to one discussed in detail in an earlier publication.[1] In short, the procedure is as follows. Fixing an energy E, the logarithmic derivatives of the reduced radial wave functions are computed for each open channel with an assumed common phase shift δ, i.e.,

$$b_c=[rf_c'(kr)/f_c(kr)]_{r=a}. \tag{25}$$

The matching radius a is chosen as small as possible, consistent with the requirements of channel orthogonality, as discussed earlier.[1] For neutral particles, f_c is given by

$$f_c(x)=(x/k)[\cos\delta j_l(x)-\sin\delta n_l(x)], \tag{26}$$

where $x=kr$. For charged particles the spherical Bessel functions are replaced by Coulomb functions. With these boundary conditions the eigenstates of the nuclear Schrödinger equation are found for the inside region, i.e., for $r\leq a$. We call the eigenvalues $E_\lambda(\delta)$. The eigenphases δ_α then are found from the condition

$$E_\lambda(\delta_\alpha)=E. \tag{27}$$

The roots of this equation can, for example, be found by a graphical method or an iteration procedure. Equation (27) has as many, in general, nondegenerate solutions as there are open channels, *viz.* N. The discussion of the problems which appear in the computation of the eigenchannels, in particular the choice of a complete orthonormal set of wave functions obeying the different boundary conditions b_c, Eq. (25), in the different channels at a given phase δ, can be taken over completely from Ref. 1.

In practice the solution of (27) is rather simple since it is only necessary to check whether one eigenvalue of the Hamiltonian matrix coincides with the energy E. This can be done simply by computing the determinant

of the matrix $H-E$. If this determinant vanishes H has an eigenvalue E. Only then does one compute the eigenvector to this eigenvalue, which then requires only a matrix inversion and not a diagonalization. The main computational effort thus lies in the determination of the wave functions and the matrix elements.

This essentially completes the computation of the eigenchannels. Namely, the nuclear wave function corresponding to the eigenvalue α can now be written in the asymptotic region, i.e., $r \approx a$, in the form (6). This involves a projection with $\tilde{\psi}_c^*$, at which point the channel orthogonality requirement[9] enters, *viz.* the relation

$$\int \tilde{\psi}_c^* \tilde{\psi}_{c'} \, dS = \delta_{cc'} \tag{28}$$

must hold with sufficient accuracy. This way the channel wave function for the channel c is split off and the amplitude $V_c^{(\alpha)}$ can be read from Eq. (6) by inspection. As a final step, the amplitudes $V_c^{(\alpha)}$ must be normalized.

The generalized natural boundary conditions discussed in the Introduction now are seen to be given by (25) when computed with an eigenphase δ_α. Thus, at each energy there exist N, in general, different natural boundary conditions.

V. RESONATING AND NONRESONATING PROCESSES

An isolated sharp resonance can be described by a one-level Breit-Wigner formula. As a matter of fact, the possibility of a description by such a Breit-Wigner formula can even be used as the defining condition for a sharp resonance. In terms of the eigenchannel description of the S matrix one sees that the simplest, nondegenerate situation which leads to such a resonance is that in which the eigenphase in one eigenchannel changes rapidly by about $\pi/2$ over an energy interval $\Delta E = \Gamma$ while all other parameters remain essentially constant over this energy region. The contributions of all other eigenchannels then can be collected into an essentially constant "background" term. Then an S-matrix element has the form

$$S_{cc'} \approx V_c^{(\alpha)} e^{2i\delta_\alpha} V_{c'}^{(\alpha)*} + B_{cc'}, \tag{29}$$

and, writing for the diverse amplitudes their absolute values and phases, the cross section is proportional to

$$\begin{aligned}\sigma_{cc'} \propto |S_{cc'}|^2 &= |V_c^{(\alpha)}|^2 |V_{c'}^{(\alpha)}|^2 \\ &+ |B_{cc'}|^2 + 2|B_{cc'}| \, |V_c^{(\alpha)}| \, |V_{c'}^{(\alpha)}| \\ &\times \cos(\varphi_B - \varphi_c + \varphi_{c'} - 2\delta_\alpha),\end{aligned} \tag{30}$$

which indeed shows a sharp peak for the discussed conditions. Since $\varphi_c - \varphi_{c'} = 0$ which can be seen from (6), the peak will occur at $\delta_\alpha = \pi/2$ if the phase $\varphi_{B_{cc'}} = \pi$. For such a situation evidently it should not be necessary to compute all eigenchannels. We shall return to this point later.

In the general case no single resonance dominates the cross section. The same holds for the eigenchannels. Then all eigenchannels have to be computed and no simplifications are possible in the description. Naturally, it still is possible to perform a meromorphic expansion for the different cross sections $\sigma_{cc'}$ as a function of the energy. However, the usefulness of such an expansion is questionable for higher level densities. Firstly, because the number of needed resonance parameters is then very large, viz., positions and residua of all poles for each partial cross section. Secondly, a nonresonating background term, an entire function of the energy, also has to be accounted for in addition. In any case, the numerical methods proposed in this paper in practice would not allow the performing of any "exact" mathematical operations which would be needed to distinguish a maximum in the entire background function from a maximum resulting from a pole since in our case only the cross sections are known as a function of energy, and only as a table of numbers of limited accuracy at that. We do not want to claim, however, that there might not exist cases where such an expansion could be of interest. For example, some poles may appear at the same position in all partial cross sections, while others may be associated only with some channels. In any case, our aim is limited to the actual computation of cross sections, at least for the time being.

Finally, one or two words are in order concerning the connection of the eigenchannel treatment with the earlier formalisms. The nuclear Schrödinger equation can be solved with arbitrary boundary conditions. We are here limiting ourselves to standing-wave solutions. Each solution of the inside problem in general will be a linear combination of all eigenchannel wave functions. The expansion in terms of the eigenchannel wave functions will thus in general involve all eigenchannels and will converge uniformly except at the matching boundary. However, for the special case of natural boundary conditions the expansion will contain only those eigenchannel wave functions which are associated with the employed natural boundary conditions, i.e., here one solution coincides with, in general, one eigenchannel wave function. In other words, here the obtained solution does not span the complete function space, and therefore not all the information concerning the nuclear system is contained in the wave function.[8] It thus seems that in the Wigner-Eisenbud procedure either one has an incomplete solution or one is saddled with the problem of non-uniform convergence at the boundary.

However, if the obtained solution dominates the reaction, as it is the case in a narrow isolated resonance, then the information contained in the dominant eigenchannel wave function should suffice for the description of this resonance, i.e., it should yield position, width, and branching ratios. That this is actually the case,

[9] A. M. Lane and R. G. Thomas, Rev. Mod. Phys. **30**, 257 (1958).

one sees by going to a neighboring energy where the boundary conditions are not the natural boundary conditions any more. There the Wigner-Eisenbud procedure works since the wave function spans the complete function space. The obtained one-level Breit-Wigner cross section can then be calculated at this energy, and one sees that one can go with the energy through the point of the natural boundary conditions without encountering any problems. This procedure works only as long as the cross section is describable by a one-level formula. In general at the point of the natural boundary conditions indeterminacies will show up. This case has been discussed in Sec. III at length.

Concluding, we believe that the proposed method is particularly suited to the actual computation of cross sections because it leads, without the consideration of intermediate auxiliary quantities, directly to the S matrix. Also, the calculational effort needed for the solution of the nuclear problem seems to us to have been minimized.

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Scattering of 40.5-MeV Alpha Particles by C^{12}, C^{13}, N^{14}, N^{15}, O^{16}, and O^{18}†

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Elastic and inelastic scattering of 40.5-MeV α particles from targets of C^{12}, C^{13}, N^{14}, N^{15}, O^{16}, and O^{18} was studied. Angular distributions were measured for a large number of excited states. It was found that the shape of the angular distribution depends on the nature of the single-particle transition involved. Six examples of quadrupole transitions involving promotion of a $p_{3/2}$ nucleon to the $p_{1/2}$ shell were found. Although the cross sections varied over a tenfold range, the shapes of the angular distributions remained very similar. Six examples of the dipole transition $p_{1/2} \rightarrow 2s_{1/2}$ and seven examples of the octupole transition $p_{1/2} \rightarrow d_{5/2}$ were also observed. The dipole transitions gave angular distributions of a characteristic and unusual shape. Excitation of the N^{14} levels at 9.41, 9.71, 10.22, and 10.55 MeV suggests that they are all $T=0$. The levels at 6.05, 6.70, 7.40, and 7.60 MeV were not observed; probably they do not exist. A weak level at 10.85 MeV and two strongly excited levels (or groups of levels) at 11.3 and 12.9 MeV were observed in N^{14}. The angular distribution of particles scattered from the 4.45-MeV level of O^{18} suggests strongly that this level is $1-$ rather than $3+$. Several unnatural parity states were observed, but no states known to have isotopic spin different from the ground state. The angular distributions for several scattered particle groups were compared with distorted-wave Born approximation calculations and very approximate reduced transition probabilities for excitation of the levels were obtained. For the quadrupole and octupole excitations the results are in reasonably good agreement with values measured by electromagnetic methods.

I. INTRODUCTION

THE inelastic scattering of α particles is a useful method for studying the surface shapes of medium-mass nuclei.[1] The levels most strongly excited are the $2+$, $4+$, and $3-$ collective states. It is therefore for the excitation of such levels that most of the angular distributions of scattered particles have been measured. The shapes of the angular distributions are determined by the angular momentum transfer L, while the absolute value of the differential cross section depends upon the collective strength of the level excited.

The light nuclei present many opportunities for studying inelastic scattering of α particles from targets for which the structure of the initial and final nuclear states is rather well understood. In many cases the transitions should be almost pure single-particle rather than collective. Large numbers of levels are sufficiently well separated in energy to permit resolution of the corresponding groups of scattered particles.

In the present survey experiment, elastic and inelastic

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[1] J. S. Blair, Phys. Rev. 115, 928 (1959).