The Reaction Matrix in Nuclear Shell Theory

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The Reaction Matrix in Nuclear Shell Theory

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§1. Introduction

In these lectures I shall discuss the nuclear shell model as a link between the properties of complex nuclei and the free-nucleon interaction. This of course is only one aspect ⁽¹⁾ of the shell model. Another is purely phenomenological; the shell model provides a framework within which many of the observed properties of nuclei have been correlated and interpreted. During this process of correlation and interpretation a vast body of mathematical technique, empirical fact and traditional practice has developed ⁽²⁾; this lore is called phenomenological nuclear shell theory. These lectures not only derive a version of the shell model from nuclear many-body theory but also compare and contrast this version of the shell model with phenomenological shell theory.

The discussion falls into three parts. First, the necessary formal framework is developed in §§2—5. An eigenvalue problem in a finite shell-model vector space is derived from many-body theory, equations are given for the effective interaction in the model space and the problem of separating core and valence properties is discussed. Second, §§6—9 concern the application of the effective-interaction formalism to the calculation of nuclear level properties.

Attention is focussed on the nuclei O^{18} and F^{18} . This part of the lectures constitutes a critical review of recent work on 'the shell model with realistic interactions.' Third, §§10—13 examine the practices of phenomenological shell theory, in particular the manner in which phenomenological effective interactions are defined. These practices are compared with the version of the shell model derived in §§2—5 and applied to nuclear level properties in §§6—9. Some of the implications of this comparison for future work in nuclear shell theory are discussed.

The basic step in calculating the properties of complex nuclei in terms of the free-nucleon interaction is the replacement of this interaction by a Brueckner reaction matrix. It has been known since the

early days of Brueckner theory that the reaction matrix is a suitable lowest-order approximation to the effective shell-model interaction. These lectures, in fact, are an essay on the reaction matrix in nuclear shell theory. This essay states the approximations under which the effective shell-model interaction reduces to a reaction matrix, discusses corrections to these approximations and reviews applications of the reaction-matrix formalism to the calculation of nuclear level-properties. Techniques for calculating reaction matrices are outside the scope of these lectures; they are discussed by Baranger in his lecture-course on 'the theory of finite nuclei' at this summer school.

§ 2. The Assumptions and Aims of Nuclear Shell Theory

The nuclear many-body problem in question here is a very restricted one. Before nuclear shell theory takes its first step two basic assumptions must be made—first, that only nucleon co-ordinates need be introduced and second, that the interaction between nucleons is a two-body interaction. The first assumption is clearly invalid whenever the energy involved is sufficient to produce real mesons; even at considerably lower energies it can have only approximate validity. Thus any nuclear theory that ignores meson co-ordinates is of necessity a low-energy approximation; this circumstance suggests that as a further approximation the nucleon motions should be treated non-relativistically.

The assumptions in question are not based on compelling *a priori* evidence. They are made, rather, as a matter of convenience (or perhaps of dire necessity) to permit a description of the nucleus as a non-relativistic system of nucleons held together by two-body forces. Comparison with experiment should then reveal to what extent and under what circumstances the underlying assumptions are valid. This comparison with experiment, of course, involves solution of the many-nucleon problem—a task which by its very nature can only be carried out approximately. The level of approximation so far achieved is largely unassessed but is certainly too crude to shed much light on the basic postulates. It can at least be said, however, that no clear violations of

the underlying assumptions have yet been found in the low-energy domain, although this circumstance may owe more to the crudity of the many-body approximations than to the accuracy of the assumptions.

Granted these basic assumptions, nuclear shell theory aims at a description of the properties of complex nuclei in terms of the forces between free nucleons. This it seeks to do in two stages. First, a single-particle potential absorbs as much as possible of the interaction between nucleons. Second, the many-body problem of interacting nucleons in a common potential is made tractable by truncation; the complete many-body Schrödinger equation is replaced by a substitute, wherein an effective Hamiltonian operates in a finite-dimensional model space.

It is of course impossible to reproduce within a finite-dimensional vector space all the aspects of a many-body problem. A lot of information (most of it useless) must be thrown away. Thus shell model wave functions are not attempts to approximate true nuclear wave functions⁽³⁾. The shell model, in fact, is an exercise in information disposal. The model space and the effective Hamiltonian must be chosen such that the information discarded is uninteresting while that retained permits a satisfactory description of the low-energy level properties of nuclei.

§ 3. The Single-Particle Potential and the Model Space of Shell Theory

The nucleus is to be treated as a non-relativistic system of nucleons held together by two-body forces; the Hamiltonian of such a system is

$$H = \sum_{i=1}^A T_i + \sum_{i < j=1}^A \bar{V}_{ij} \quad (1)$$

where A is the number of nucleons, T_i is the kinetic energy of the i 'th nucleon and $\bar{V}_{ij}$ is the interaction potential between free nucleons.

The shell model⁽⁴⁾ starts by absorbing as much as possible of the interaction $\bar{V}$ between nucleons in a single-particle potential U . The Hamiltonian of eq. (1) can be rewritten in a form which reflects this separation of the effects of interaction;

$$\left. \begin{aligned}
 H &= H_0 + V \\
 H_0 &= \sum_{i=1}^A (T_i + U_i) \\
 V &= \sum_{i < j=1}^A \bar{V}_{ij} - \sum_{i=1}^A U_i
 \end{aligned} \right\} \quad (2)$$

where H_0 is the single-particle shell-model Hamiltonian and V is the residual interaction between nucleons — residual in the sense that it is the part of the two-body interaction not included in the single-particle potential U .

In a complete many-body treatment of shell theory, the single-particle potential is determined by some variant of the Hartree-Fock procedure⁽⁵⁾; potentials constructed in this way are in general non-local. Most shell-model studies⁽⁴⁾ use a phenomenological local approximation to the HF potential, of the form

$$U = U(r) + \xi \vec{l} \cdot \vec{s} \quad (3)$$

with central (harmonic oscillator or Woods-Saxon) and spin-orbit components. The shape and depth of $U(r)$ and the strength ξ of the spin-orbit force are adjusted so that the spectrum of H_0 (Fig. 1) reproduces the observed single-particle level systematics of nuclei. All the shell-model studies discussed in these lectures use the local single-particle potential of eq. (3) with a harmonic-oscillator central component.

The eigenfunctions of $H_0(i)$ yield a complete set $\{\phi^{n\ell j}_{mt_z}(\vec{r}_i, \sigma_i, \tau_i)\}$ of single-particle states for the i 'th nucleon. Each such state is labelled by its charge ($\frac{1}{2} - t_z$), its principal quantum number n , its orbital angular momentum ℓ and its total spin quantum numbers (j, m) . Totally antisymmetric A -particle states can be constructed as linear combinations of Slater determinants. As their constituent single-particle wave functions $\phi^{n\ell j}_{mt_z}$ run over all orbits, the determinants span the complete Hilbert space D of the system. The dimensions of D exceed all bounds.

Now a many-body problem cannot be solved simply by rewriting its Hamiltonian and choosing a suitable basis in its Hilbert space. Shell theory faces this situation with a characteristic act of truncation; the intractable problem of the true Hamiltonian acting in the infinite-dimensional Hilbert space D is replaced by that of a modified or effective Hamiltonian H_{eff} acting in a finite model space d . This model space must have enough life left in it to describe the salient features of low-lying nuclear states.

Thus a shell-model calculation starts with a truncation. Methods of carrying out this truncation rely on the fact that U has been chosen to make the extreme single-particle model as good as possible. To discuss anything more than ground-state spins and moments, of course, more than one nucleon must be given an active role. Yet the single-particle model is so successful ⁽⁴⁾, that its extreme requirements ought clearly to be relaxed rather than abandoned completely.

A procedure therefore emerges for the construction of shell-model vector spaces. All but a few of the A nucleons remain undisturbed in completely filled orbits to form an inert core; the few remaining valence nucleons are permitted to enter only a few of the available single-particle orbits. Let there be n valence nucleons and μ active orbits; further, let the active orbits be labelled in abbreviated fashion by their total angular momentum quantum numbers $j_1, j_2, \dots, j_\mu$. Then the model space d is the finite vector space spanned by a complete set of antisymmetric n -particle states of the configurations $(j_1, j_2, \dots, j_\mu)^n$. If each basis state is such a linear superposition of Slater determinants that its total angular momentum J is specified, then the model space d splits into a direct sum of disjoint J -subspaces d_J . The truncation procedure is illustrated in Fig. 2. The J -decomposition is symbolized by

$$(j_1, j_2, \dots, j_\mu)^n \Rightarrow d = d_{J_1} \oplus d_{J_2} \oplus \dots \oplus d_{J_{\text{max}}} \quad (4)$$

Consider as an example the nucleus ${}^{18}_{8}\text{O}_{10}$. The pertinent single-particle levels appear at the bottom of Fig. 1. In the simplest shell-model description of low-lying states in O^{18} , 8 of the neutrons and all 8 protons fill the $1s_{\frac{1}{2}}$, $1p_{\frac{3}{2}}$ and $1p_{\frac{1}{2}}$ orbits to form an inert O^{16} core. Since of the first few extra-core orbits $1d_{\frac{5}{2}}$ lies considerably above $1d_{\frac{3}{2}}$ and $2s_{\frac{1}{2}}$, attention can be confined to $1d_{\frac{5}{2}}$ and $2s_{\frac{1}{2}}$ orbits. The model space for O^{18} is therefore spanned by the states of the configurations $(1d_{\frac{5}{2}}, 2s_{\frac{1}{2}})^2$;

$$d(\text{O}^{18}) = d_0 \oplus d_2 \oplus d_3 \oplus d_4$$

$$d_0 = \{(1d_{\frac{5}{2}})^2_0, (2s_{\frac{1}{2}})^2_0\}$$

$$d_2 = \{(1d_{\frac{5}{2}})^2_2, (1d_{\frac{5}{2}}2s_{\frac{1}{2}})_2\} \quad (5)$$

$$d_3 = \{(1d_{\frac{5}{2}}2s_{\frac{1}{2}})_3\}$$

$$d_4 = \{(1d_{\frac{5}{2}})^2_4\}$$

The model space for O^{18} is therefore 6-dimensional.

Once the model space has been chosen, an effective Hamiltonian must be determined to act in it. This problem will be discussed in §§ 4 and 5. The matrix of the Hamiltonian is then constructed and diagonalized within the n-particle basis chosen to span the model space; construction and diagonalization of the energy matrix is of course equivalent to solution of the Schrödinger equation within the model space. Diagonalization of the energy matrix proceeds separately in each of the fixed-J subspaces d_J of the model space; thus in the case of O^{18} within $(1d_{\frac{5}{2}}, 2s_{\frac{1}{2}})^2$ the largest matrices to be diagonalized are the 2×2 matrices for $J = 0$ and 2 although the total dimension of the model space is 6.

It is clear that this procedure of constructing and diagonalizing the complete energy matrix within d is feasible only if the dimensions involved are quite small. In fact it is well known that very few active orbits and very few valence nucleons are needed to produce catastrophically large dimensions. Imagine for example trying to construct all the isobaric-spin $T = 3$ states of the nucleon configurations $(1f_{7/2}, 2p_{3/2}, 2p_{1/2}, 1f_{5/2}, 1g_{9/2})^{20}$; this problem would be of great interest in providing a good model description of $^{60}_{28}\text{Ni}_{32}$ where it is not physically desirable to assume an inert Ni^{56} core (which eliminates the $1f_{7/2}$ shell and 16 of the 20 valence nucleons) or to ignore the $1g_{9/2}$ orbit. The dimensions involved run into the hundreds of thousands.

The dilemma here is characteristic of the shell model. For all but a few specially simple—or specially simplified—problems, exact diagonalization of the complete model energy matrix is out of the question. In fact, nearly all interesting shell-model calculations are impossible; the spectacular developments in modern computer technology have had remarkably little impact on this situation. The main focus of interest in shell-model technique must of necessity be the development and assessment of approximation methods.

To conclude this section, consider in more detail the nature of the act of truncation ⁶ whereby the complete Hilbert space D of the A -particle system is reduced to the finite n -particle model space d of the configurations $(j_1 j_2 \dots j_\mu)^n$. The first step is to introduce the eigenstates $|\Phi_i\rangle$ of H_0 as a basis in D ; the basis states therefore satisfy the equation

$$H_0 |\Phi_i\rangle = \epsilon_i |\Phi_i\rangle. \quad (6)$$

Each basis state will be assumed to have definite values of the total angular-momentum quantum numbers (JM) and to belong to a definite configuration $j_1^{n_1} j_2^{n_2} \dots j_\mu^{n_\mu}$ ($\sum n_k = n$). Such states can be built as

linear superpositions of Slater determinants.

$$\det. |a_1 a_2 \dots a_A| = \prod_{i=1}^A c_{a_i}^+ |0\rangle \quad (7)$$

where a denotes a set (jm) of single-particle labels, c_a^+ creates a nucleon in a state a and $|0\rangle$ is the no-particle or vacuum state. The determinantal expansion of the basis state $|\Phi_i\rangle$ can then be written in the form

$$|\Phi_i(JM)\rangle = \sum_r C_{ir} \det_r |a_1 a_2 \dots a_A| \quad (8)$$

where r runs over all distributions $\{m_1 m_2 \dots m_A\}$ of magnetic quantum numbers consistent with the orbit-distribution $\{j_1 j_2 \dots j_A\}$ of the configuration under consideration and with the constraint $\sum_k m_k = M$.

Now the model space d is made by confining the first $(A-n)$ nucleons to the lowest accessible single-particle orbits, thereby forming a closed-shell core; denote the $(A-n)$ -particle core determinant by $|\Psi_c\rangle$. Then d is spanned by those states $|\Phi_i\rangle$ ($i \in d$) whose constituent determinants (eq. 8) are of the form

$$\det_{r \in d} |a_1 \dots a_A| = \left(\prod_{k=1}^n c_{a_k}^+ \right) |\Psi_c\rangle \quad (9)$$

where the states a_k ($k = 1$ to n) of the valence nucleons belong to the active orbits $j_1, j_2, \dots, j_\mu$.

The n -particle states of the configurations $(j_1 j_2 \dots j_\mu)^n$ are thus in reality A -particle states with $A-n$ particles confined to a closed-shell core. Phenomenological nuclear shell theory has proceeded on the assumption that, while the core strongly influences the total energies of nuclear states, excitation energies are determined by the valence nucleons. The core influences the properties (other than the total energy) of low-lying levels only by modifying the effective interaction and the operators that determine moments and transition rates.

§4. Equations for the Effective Interaction

Suppose that a finite model space d has been chosen for the A-particle nucleus under consideration. An effective-interaction Hamiltonian

$$H_{\text{eff}} = H_0 + V_{\text{eff}} \quad (10)$$

within the model space must now be determined. The procedure followed here was suggested twelve years ago by Eden and Francis;⁽⁷⁾ its basic equations are due to Bloch and Horowitz.⁽⁸⁾

The shell-model Hamiltonian H_{eff} is to be chosen such that its lowest eigenvalues coincide with those of the true Hamiltonian. This energy requirement is not in itself enough to determine H_{eff} ; some restriction must be placed on the corresponding eigenvectors. A sufficient additional demand is that the model eigenvector $|\Psi_d\rangle$ corresponding to the eigenvalue E is simply the projection on the model space of the true eigenvector $|\Psi\rangle$. In other words, the effective shell-model interaction is to be determined such that, in an eigenvalue problem within the model space, it reproduces some of the lowest eigenvectors of the complete Hamiltonian of the system. The embedding process involved may be symbolized as follows:

$$\left\{ \begin{array}{l} H |\Psi\rangle = E |\Psi\rangle \\ \text{in } D \end{array} \right\} \Rightarrow \left\{ \begin{array}{l} H_{\text{eff}} |\Psi_d\rangle = E |\Psi_d\rangle \\ \text{with } |\Psi_d\rangle = P |\Psi\rangle \\ \text{in } d \end{array} \right\} \quad (11)$$

where P [eq. (12)] projects on to the model space d .

This embedding procedure leads directly to equations for $|\Psi_d\rangle$ and for V_{eff} . To derive these equations, it is convenient to proceed in the manner outlined in §3 and to introduce the eigenstates $|\Phi_i\rangle$ of the single-particle Hamiltonian H_0 as basis states in the complete Hilbert space D of the system; the states $|\Phi_i\rangle$ which lie in d span the model

space. The operator P that projects on to d and the complementary operator Q that projects out of d are then given by

$$\left. \begin{aligned} P &= \sum_{i \in d} |\Phi_i\rangle \langle \Phi_i| \\ Q &= \sum_{i \notin d} |\Phi_i\rangle \langle \Phi_i| \\ P + Q &= I \end{aligned} \right\} \quad (12)$$

where I is the unit operator in D . Expanded in the single-particle basis the eigenvector $|\Psi\rangle$ becomes

$$|\Psi\rangle = \sum_{i \in D} a_i |\Phi_i\rangle \quad (13)$$

while the corresponding model eigenvector is

$$|\Psi_d\rangle = P |\Psi\rangle = \sum_{i \in d} a_i |\Phi_i\rangle. \quad (14)$$

The Schrödinger equation for $|\Psi\rangle$ is

$$(E - H_0) |\Psi\rangle = V |\Psi\rangle. \quad (15)$$

The expansion (13) then yields

$$\sum_{j \in D} (E - \epsilon_j) a_j |\Phi_j\rangle = V |\Psi\rangle \quad (16)$$

and alternatively

$$(E - \epsilon_i) a_i = \langle \Phi_i | V | \Psi \rangle \quad (17)$$

on taking the scalar product with $|\Phi_i\rangle$ and using the assumed orthonormality of the basis. Eq. (17) holds for all $i \in D$.

Eq. (17) is simply a restatement of the Schrödinger equation for $|\Psi\rangle$. It is however a useful restatement since it suggests an immediate solution to the embedding problem symbolized by (11). In fact, such a solution would be provided by an operator V_{eff} satisfying the equations

$$(E - \epsilon_i) a_i = \langle \Phi_i | V_{\text{eff}} | \Psi_d \rangle \quad (18)$$

for all $i \in D$. It would then follow that, just as the set of eqs. (17) for all $i \in D$ expresses the Schrödinger equation for the true eigenvector $|\Psi\rangle$, so also the subset of eqs. (18) for $i \in d$ would specify an eigenvalue problem of the desired sort in the model space d —an eigenvalue problem, specifically, for the operator H_{eff} of eq. (10) with eigenvalue E and eigenvector $|\Psi_d\rangle$.

Now it is clear that eq. (18) is true for any operator V_{eff} for which

$$V_{\text{eff}} |\Psi_d\rangle = V |\Psi\rangle. \quad (19)$$

Such an operator maps d into D and must therefore have non-zero matrix elements $\langle \Phi_i | V_{\text{eff}} | \Phi_j \rangle$ with both $i \in d, j \in d$, and also with $i \notin d, j \in d$. To derive the equations for V_{eff} implied by eq. (19) note first that

$$\begin{aligned} \frac{Q}{E - H_0} V |\Psi\rangle &= \sum_{i \notin d} \frac{|\Phi_i\rangle \langle \Phi_i | V |\Psi\rangle}{E - \epsilon_i} \\ &= \sum_{i \notin d} a_i |\Phi_i\rangle \\ &= Q |\Psi\rangle \end{aligned} \quad (20)$$

where the successive steps use eq. (12), eq. (17), and again eq. (12).

This alternative form for the projection operator Q can be used to recast the basic requirement (19);

$$\begin{aligned}
V_{\text{eff}} |\Psi_d\rangle &= V |\Psi\rangle \\
&= V(P + Q) |\Psi\rangle \\
&= V |\Psi_d\rangle + V \frac{Q}{E - H_0} V |\Psi\rangle \\
&= \left\{ V + V \frac{Q}{E - H_0} V_{\text{eff}} \right\} |\Psi_d\rangle, \quad (21)
\end{aligned}$$

where the second step uses eq. (12), the third eqs. (14) and (20), and the last eq. (19) itself. The desired equation for V_{eff} is thus

$$V_{\text{eff}}(E) = V + V \frac{Q}{E - H_0} V_{\text{eff}}(E) \quad (22)$$

where the fact that V_{eff} depends on the eigenvalue E has been indicated explicitly. This equation for V_{eff} is sufficient in the sense that any operator that satisfies it will also satisfy eq. (19) and hence will also yield the eigenvalue problem expressed by eqs. (18).

The desired shell-model eigenvalue problem, the outcome of the embedding process symbolized by (11), is therefore given by eqs. (18) and (22); let these equations be rewritten in terms of the basis spanned by the eigenstates $|\Phi_i\rangle$ of H_0 . The model eigenvector $|\Psi_d\rangle$ is determined, through eq. (14), by the secular equations

$$(E - \epsilon_i) a_i = \sum_{j \in d} \langle \Phi_i | V_{\text{eff}}(E) | \Phi_j \rangle a_j \quad (23)$$

which hold for all $i \in D$. The matrix elements of the effective interaction satisfy

$$\begin{aligned}
\langle \Phi_i | V_{\text{eff}}(E) | \Phi_j \rangle &= \langle \Phi_i | V | \Phi_j \rangle \\
&+ \sum_{k \notin d} \frac{\langle \Phi_i | V | \Phi_k \rangle \langle \Phi_k | V_{\text{eff}}(E) | \Phi_j \rangle}{E - \epsilon_k} \quad (24)
\end{aligned}$$

for all $i \in D$ and for $j \in d$. Eqs. (23) and (24) are the basic equations of shell theory.

Equations (23) and (24) are simply another restatement of the Schrödinger equation (15) for $|\Psi\rangle$. This Schrödinger equation has, in a sense, been split into two parts, one within the model space, the other outside it.

1) For $i \in d$, eqs. (23) and (24) define an eigenvalue problem within d for the energy E and the corresponding model eigenvector $|\Psi_d\rangle$, the projection $P|\Psi\rangle$ of $|\Psi\rangle$ in d .

2) For $i \notin d$, eqs. (23) and (24) yield the component $Q|\Psi\rangle$ of $|\Psi\rangle$ outside d , thereby completing the determination of $|\Psi\rangle$. $|\Psi\rangle$ (and therefore $|\Psi_d\rangle$) is determined only to within normalization; this does not influence the calculation of energies but is of course crucial in the treatment of moments and transition rates. It will be assumed that the normalization is such that

$$\langle \Psi | \Psi_d \rangle = \langle \Psi_d | \Psi_d \rangle = 1. \quad (25)$$

This choice of normalization is possible only if $|\Psi\rangle$ has a non-vanishing component within the model space d —an assumption which is implicit in the entire discussion of this section since it is manifestly impossible to discuss an eigenstate in terms of a model space to which it is orthogonal.

When i is restricted to values lying in d , eq. (23) has the general form of a shell-model secular equation. It differs, in fact, from the usual shell-model secular equation in two important respects. First, the energy E is the total energy of the state in question rather than the interaction energy of the valence particles; removal of the core energy will be discussed in §5. Second, the effective interaction depends explicitly on the desired energy eigenvalue E .⁽⁹⁾ This E -dependence couples equations (23) and (24). Bloch and Horowitz⁽⁸⁾ prove that, in spite of the E -dependence, eqs. (23) and (24) have exactly d real roots, where d is the dimension of the model space. The model eigenvectors $|\Psi_d\rangle$ corresponding to different roots are not necessarily orthogonal since they are eigenvectors of different Hamiltonians $H_{\text{eff}}(E)$.

No quantitative studies have been reported of this state-dependence of the effective interaction. The procedure has been to replace the eigenvalues E in the energy denominator of eq. (24) by a suitable average; the same effective interaction is then obtained for all eigenstates in the model space and eqs. (23) and (24) decouple. This averaging process is reasonable only if the excitation energies $E - \epsilon_k$ of all important states $|\Phi_k\rangle$ in eq. (24) are large compared with the total spread or variation in the desired eigenvectors E .

This approximation tends to break down whenever the model space is forced to accommodate states of widely different degrees of configuration purity, where of course, the pure configurations in question are those of the model space d . To take a specific example, suppose that a set of states $|\Psi^r\rangle$ has been selected for consideration in a shell-model study within a certain model space d . These eigenvectors can be written in the form

$$|\Psi^r\rangle = \alpha_r |\Psi_d^r\rangle + \beta_r |\Psi_e^r\rangle + \dots \quad (26)$$

where $|\Psi_d^r\rangle$ is the model eigenvector and $|\Psi_e^r\rangle$ is the component of $|\Psi^r\rangle$ in configurations bordering on d . In the case of O^{18} , if d is the space spanned by the configurations $(1d, 2s)^2$, e might involve the $4p, 2h$ configurations $[1p^{-2}, (1d, 2s)^4]$. The quantity $|\beta_r/\alpha_r|$ measures the degree of configuration purity of the state $|\Psi^r\rangle$; a small value of $|\beta/a|$ implies a high degree of purity against excitations into the configurations e . Suppose, then, that one of the states $|\Psi^r\rangle$, call it $|\Psi^0\rangle$, is much less pure than all the others; suppose, in other words, that $|\beta_0/\alpha_0| \gg 1$ while $|\beta_r/\alpha_r| \ll 1$ for all $r \neq 0$.

If the model space has been chosen sensibly, the unperturbed single-particle energies $\epsilon_k^{(e)} = \langle H_0 \rangle_{k \in e}$ for the states $|\Phi_k\rangle$ belonging to the configurations e are such that all the energy-differences $E^r - \epsilon_k$ are large relative to the spread in the desired eigenvalues E^r . Thus the criterion given

above for the neglect of state-dependence in V_{eff} would seem to be fulfilled. However, large values for the energy differences $E^r - \epsilon_k$ also imply small admixtures of the unperturbed states $|\Phi_k\rangle$ ($k \in e$) in the eigenvectors $|\Psi^r\rangle$. It is then clear that $|\Psi^0\rangle$ can acquire its large configuration impurity only if $|\Psi_e^0\rangle$ is a strongly collective state whose energy expectation-value $\langle H_0 + V \rangle_e^0$ is depressed far below its single-particle energy $\langle H_0 \rangle_e^0$. The situation is illustrated in Fig. 3. The contribution of this collective state to the Pauli operator $Q/E - H_0$ in eq. (22) or (24) is

$$\begin{aligned} & \frac{|\Psi_e^0\rangle\langle\Psi_e^0|}{E - \langle H_0 \rangle_e^0} \left\{ 1 + \frac{\langle V \rangle_e}{E - \langle H_0 \rangle_e^0} + \left(\frac{\langle V \rangle_e}{E - \langle H_0 \rangle_e^0} \right)^2 + \dots \right\} \\ & = \frac{|\Psi_e^0\rangle\langle\Psi_e^0|}{E - \langle H_0 + V \rangle_e^0}. \end{aligned} \quad (27)$$

The result follows by expanding the states $|\Phi_k\rangle$ ($k \in e$) in terms of the states $|\Psi_e^r\rangle$ (and of enough other states of the configurations e to make a complete set), isolating the contribution of $|\Psi_e^0\rangle$, iterating, and summing a geometric series. The energy denominator in eq. (27) now involves the energy expectation-value $\langle H_0 + V \rangle_e^0$ which lies in the middle of the desired eigenvalues E^r and, presumably, especially close to E^0 . Thus the variation in the denominator $(E^r - \langle H \rangle_e^0)^{-1}$ with E^r is certainly not small compared with the spread in the desired eigenvalues E^r . The argument given above for neglecting the E -dependence of V_{eff} therefore breaks down. To summarize, state-dependent effects can be expected to be large whenever, in the midst of energy levels to be treated within a certain model space d , there lies a highly collective state arising predominantly from higher configurations.⁽¹⁰⁾

Clearly such state-dependent effects can and should be minimized by suitable choice of model space d . If a certain state demands a very different model interaction from its neighbors, the remedy is obviously to enlarge the model space. This of course may be difficult or impossible to do because of the dimension problems mentioned in §3.

From now on the state-dependence of the interaction will be neglected. As in all studies so far published, the eigenvalue E in eq. (24) will be replaced by a suitable average energy $\bar{E}$. An approximate state-independent interaction $V_{\text{eff}} = V_{\text{eff}}(\bar{E})$ therefore emerges.

The problem of state-dependence has now been turned aside although it certainly has not been solved. It is in fact clear that E -dependence of the Hamiltonian is an inescapable property of the embedding procedure under consideration; no single Hermitian Hamiltonian can exist which will have all d model states as eigenvectors with eigenvalues E . For the existence of such a Hamiltonian would imply that different model eigenvectors $|\Psi_d\rangle$ are necessarily orthogonal, in conflict with the fact that the projections $|\Psi_d\rangle$ on d of orthogonal eigenvectors $|\Psi\rangle$ are not in general themselves orthogonal.

§5. Separation of Core and Valence Energies

Conventional shell-model calculations make no attempt to compute absolute energies; they deal with energies referred to the nearest closed-shell nucleus. In other words, the shell model calculates the quantity $E - E_c$ where E is the total energy of the state in question and E_c is the total ground-state energy of the closed-shell nucleus obtained by removing the valence nucleons. It is assumed that such relative energies stem entirely from the interactions of the valence nucleons with each other and with the core. Implicit in this assumption is the farther assumption that the total energy of a nuclear state is the sum of separate contributions from the core and from the valence nucleons. The separation of core and valence energies will now be discussed¹¹ from the viewpoint of the embedding formalism of § 4.

Let the secular equation (23) be restricted to the model space d and written in matrix form. The model eigenvector $|\Psi_d\rangle$ is then characterized by the column vector $\underline{a}$ whose components are the coefficients $a_i (i \in d)$ in eq. (14). Eq. (23) becomes

$$[H_0 + V_{\text{eff}}(E) - EI]_d \cdot \tilde{a} = 0 \quad (28)$$

where V_{eff} is the effective-interaction matrix, H_0 is the diagonal single-particle energy matrix and I is the unit matrix of rank d (the dimension of the model space d). The matrix elements of V_{eff} are given by eq. (24).

Eq. (28) is still not a true shell-model secular equation even when the E -dependence of V_{eff} is ignored. The energy E that it contains is the total energy of the nuclear state under consideration, including the binding energy of the closed-shell core. It remains therefore to remove the core energy E_c , the total energy of the closed-shell nucleus obtained by removing the valence nucleons.

The total energy E of the state in question is the sum of an unperturbed contribution E_0 and an energy shift ΔE due to residual interactions:

$$E = E_0 + \Delta E \quad (29)$$

It is easy to separate the core and valence parts of E_0 . To do this note first that

$$E_0 = \langle \Psi_d | H_0 | \Psi_d \rangle \quad (30)$$

The single-particle Hamiltonian H_0 can be expressed, in the chosen basis, in the form

$$H_0 = \sum_{\ell} \epsilon_{\ell} N_{\ell} \quad (31)$$

where ℓ symbolizes the quantum numbers $(n \ell j \tau)$ of a single-particle orbit, N_{ℓ} is the particle-number operator of that orbit, ϵ_{ℓ} is its single-particle energy and the sum extends over all orbits. The core part of H_0 is

$$H_{0c} = \sum_{A(\text{occ.})} \epsilon_A N_A \quad (32)$$

where the sum includes only occupied orbits A , while the valence part is

$$H_{0v} = \sum_v \epsilon_v N_v \quad (33)$$

summed over valence orbits v . The separation

$$E_0 = E_{0v} + E_{0c} \quad (34)$$

then follows on taking the expectation value of H_0 in the state $|\Psi_d\rangle$.

The energy shift ΔE must now be treated in similar fashion.

The problem at hand is therefore to give an operational definition of the core and valence terms in the energy shift

$$\Delta E = \Delta E_c + \Delta E_v \quad (35)$$

and to show how this separation — whose possibility, though plausible, is far from obvious — influences the secular equation (28) and the defining equation (24) of the effective interaction.

Start, then, from eq. (22) or (24) for the effective interaction and iterate with respect to V ;

$$\langle \Phi_i | V_{\text{eff}}(E) | \Phi_j \rangle = \sum_{p=0}^{\infty} \langle \Phi_i | V \left(\frac{Q}{E - H_0} V \right)^p | \Phi_j \rangle. \quad (36)$$

Consider, for the moment, matrix elements of V_{eff} within the model space (ied, jed). Each term in this iterated expansion can be represented by a Goldstone diagram (¹²) with $|\Psi_c\rangle$ (the core determinant) as reference-state and with n ingoing and outgoing external lines to represent valence nucleons. These diagrams, of course, differ from true Goldstone diagrams in that they contain E rather than E_0 in their energy denominators.

Three types of diagram appear in the expansion (36) and are illustrated in Fig. 4 in the special case of 3 valence particles.

- i) A core diagram is one in which none of the V-interactions is attached to an external line. The external valence lines (representing model states $|\Phi_i\rangle$, ied) propagate undisturbed. Diagram a) of Fig. 4 is a core diagram.
- ii) A valence diagram is one in which all the V-interactions are attached to external lines. Diagram b) of Fig. 4 is a valence diagram.
- iii) A mixed diagram is one in which some of the V-interactions are attached to external lines and some are not. Diagrams c) and d) of Fig. 4 are mixed diagrams.

These definitions can be restated succinctly by defining core components of a diagram as subdiagrams without external lines; thus the set of V-interactions in a core component begins and ends with the core or vacuum state $|\psi_c\rangle$. Then a diagram is a core diagram if and only if it consists entirely of core components; it is a valence diagram if it has no core components and a mixed diagram if it has both core components and V-interactions attached to external lines.

Two aspects of the perturbation expansion (36) stand in the way of a clean separation of core and valence energies:

- 1) the presence of mixed diagrams
- 2) the fact that the energy denominators in the core diagrams contain the valence energy ΔE_v and the energy denominators in the valence diagrams contain the core energy ΔE_c . These two sources of difficulty cancel each other.

No proof of this cancellation will be given here. The basic

mathematical tool (¹³) is an algebraic identity for the energy denominator e^{-1} where e splits into two parts;

$$e = e_0 + \delta e$$

$$\frac{1}{e} = \frac{1}{e_0} + \frac{1}{e_0} (-\delta e) \frac{1}{e_0} + \frac{1}{e_0} (-\delta e) \frac{1}{e_0} (-\delta e) \frac{1}{e_0} + \dots \quad (37)$$

Consider, then, a set of diagrams with energy denominators e ; substitution of the series (37) for each such denominator gives rise to a new set of diagrams, involving energy denominators e_0 and δe insertions to all orders. This procedure will be referred to as "expanding δe out of the energy denominators." The aim is to demonstrate cancellation between diagrams in the new set containing one or more δe insertions and undesirable diagrams in the original set. Such cancellation is possible because a diagrammatic expansion exists for δe itself; substitution of this expansion for each δe insertion gives rise to a host of new diagrams exactly like those in the original set except that the energy denominators e have been replaced by e_0 .

This procedure is now to be applied to the terms of the perturbation expansion (36) with energy denominators $e = E - H_0$. In the core diagrams take

$$\left. \begin{aligned} \delta e &= \Delta E_v \\ e_0 &= (E_0 + \Delta E_c - H_0) \end{aligned} \right\} \quad (38)$$

and in the valence diagrams take

$$\left. \begin{aligned} \delta e &= \Delta E_c \\ e_0 &= (E_0 + \Delta E_v - H_0) \end{aligned} \right\} \quad (39)$$

where, it will be recalled, ΔE_c and ΔE_v are yet to be defined. Thus ΔE_v is to be expanded out of the core diagrams, ΔE_c out of the valence diagrams.

The central result of this section can now be stated; with the definition of ΔE_c and ΔE_v given below, the core diagrams with at least one ΔE_v insertion and the valence diagrams with at least one ΔE_c insertion exactly cancel the mixed diagrams of the original expansion. Only two sorts of diagram survive—core diagrams without insertions and valence diagrams without insertions.

Consider next the surviving core diagrams in the expansion (36) for V_{eff} . Since in the core diagrams the external valence lines propagate undisturbed, each such diagram is proportional to the unit operator I in d . Thus the sum of all surviving core diagrams is a multiple of I —the multiplier to be determined by summing all core components. Now the energy denominators in the surviving core diagrams are $(E_0 + \Delta E_c - H_0)$; the set of all core components is therefore identical to the Brillouin-Wigner perturbation expansion for the core energy-shift ΔE_c . ΔE_c can then be expanded out of the energy denominators and the resulting diagrams with ΔE_c insertions shown to cancel the unlinked terms (¹⁴) in the original expansion for ΔE_c . (A diagram is said to be unlinked if it consists of two or more disjoint pieces.) The set of all surviving core components is therefore identical to the Goldstone linked-cluster expansion (¹⁵) for the core energy shift ΔE_c . This can now be taken as the desired definition of ΔE_c and hence, through eq. (35), of ΔE_v as well; ΔE_c is the ground-state energy shift of the core nucleus $|\psi_c\rangle$ made by removing the valence nucleons in $|\psi_d\rangle$ and is given by a Goldstone linked-cluster expansion of the usual sort with energy denominators $(E_0 - H_0)$. With this definition of ΔE_c , the core contribution to the part of V_{eff} within d is given by

$$[\text{Core part of } V_{\text{eff}}] = \Delta E_c \cdot I \quad (40)$$

where I is the unit matrix within d .

According to eq. (39), the energy denominators in the surviving valence diagrams are $(E_0 + \Delta E_v - H_0)$. Define now the total core energy E_c and the total valence energy E_v by

$$\left. \begin{aligned} E_c &= E_{0c} + \Delta E_c \\ E_v &= E_{0v} + \Delta E_v \\ E &= E_c + E_v \end{aligned} \right\} \quad (41)$$

Recall in this connection that ΔE_c is defined by the core Goldstone expansion, that ΔE_v is then defined by eq. (35) and that E_{0c} and E_{0v} are the expectation values in the state $|\psi_d\rangle$ of the operators H_{0c} and H_{0v} of eqs. (32) and (33). Thus the valence energy denominator can be rewritten

$$[E_{0v} + \Delta E_v - (H_0 - E_{0c})] = (E_v - \bar{H}_0). \quad (42)$$

Now

$$E_{0c} = \sum_{A(\text{occ})} 2\Omega_A \epsilon_A \quad (43)$$

where $2\Omega_A$ is the number of particles in the completely filled orbit A. Then since

$$N_A^h = 2\Omega_A - N_A \quad (44)$$

is the hole-number operator for orbit A,

$$\bar{H}_0 = - \sum_{A(\text{occ})} \epsilon_A N_A^h + \sum_a \epsilon_a N_a \quad (45)$$

where the sum over A includes all core orbits and the sum over a all valence and empty orbits. The valence contribution $\mathfrak{V}(E_v)$ to the effective interaction within d is thus given by summing all valence diagrams with energy denominators $(E_v - \bar{H}_0)$. The final result for V_{eff} is accordingly

$$V_{\text{eff}}(E) = \Delta E_c \cdot I + \mathfrak{V}(E_v) \quad (46)$$

where the core contribution is taken from eq. (40) and the valence contribution is given by

$$\langle \phi_i | \mathfrak{V}(E_v) | \phi_j \rangle = \sum_{p=0}^{\infty} \left\{ \langle \phi_i | V \left(\frac{Q}{E_v - \bar{H}_0} V \right)^p | \phi_j \rangle \right\}_v \quad (47)$$

Here $\bar{H}_0$ is given by eq. (45) and Q is the projection operator out of the model space d . The symbol $\{ \ }_v$ indicates that only valence terms—those without core components—are to be included in the expansion.

The argument can now be completed by substitution from eq. (46) in the secular equation (28). Noting that within d the single-particle Hamiltonian reduces to

$$H_0 = E_{0c} I + H_{0v}, \quad (48)$$

the secular equation becomes

$$[H_{0v} + \mathfrak{V}(E_v) - (E - E_{0c} - \Delta E_c) I]_d \cdot \underline{a} = 0. \quad (49)$$

The quantity in round brackets is seen from eq. (41) to be the valence energy E_v . The secular equation then assumes its final form;

$$[H_{0v} + \mathfrak{J}(E_v) - E_v I]_d \cdot a \approx 0 \quad (50)$$

where $\mathfrak{J}(E_v)$ is given by eq. (47), H_{0v} by eq. (33). Apart from the lingering dependence of $\mathfrak{J}$ on E_v , eq. (50) is now a shell-model secular equation of standard form. The desired separation of core and valence contributions to the energy has thus been achieved.

The effective interaction $V_{\text{eff}}(E)$ of § 4 has been replaced by a reduced effective interaction $\mathfrak{J}(E_v)$ from which contributions from the inert core $|\psi_c\rangle$ have been eliminated. Of course, core-excited states can occur as intermediate states in the valence diagrams that contribute to $\mathfrak{J}$. Thus only inert-core effects have been eliminated. A price has been paid for this elimination of inert-core effects. Whereas V_{eff} is expressed in § 4 as the solution of an equation (eq. (24)) of the Lippmann-Schwinger type, $\mathfrak{J}$ has been given only as the sum of a perturbation expansion (eq. (47)) in V . No non-perturbative expression for $\mathfrak{J}$ is known.

The perturbation series (47) for $\mathfrak{J}$ contains the desired eigenvalue E_v in its energy denominators; the reduced effective interaction is therefore E -dependent, as of course it must be. All the comments made in § 4 about the E -dependence of V_{eff} are equally valid here. Another point about the perturbation expansion (47) is that it contains unlinked terms; one of these (¹⁶) (for $n = 4$) is shown in Fig. 5. Morita (¹⁷) and Brandow (⁶) have shown that if true E -dependent effects (those arising from the non-orthogonality of different states $|\psi_d\rangle$) are negligible, then, on expanding ΔE_v out of the energy denominators in eq. (47), diagrams with ΔE_v insertions exactly cancel the unlinked diagrams. Thus a completely linked expansion, with energy denominators $(E_{0v} - \bar{H}_0)$, is obtained for $\mathfrak{J}$. It is obvious that this cancellation procedure merely eliminates an apparent formal E -dependence when there is no real physical E -dependence. If the state-dependence of $\mathfrak{J}(E_v)$ is not negligible, then the linked-cluster expansion defines some average energy-independent effective interaction which may well be useful as an approximation.

On this basis it will usually be sensible to include only the linked terms of the expansion (47) in computing matrix elements of $\mathfrak{g}$; state-dependent effects too large for this procedure to be accurate probably ought to be handled by explicit extension of the model space.

The effective interaction $\mathfrak{g}$ has matrix elements outside the model space d . Such matrix elements do not influence the calculation of energy eigenvalues but are necessary to determine the components of $|\Psi\rangle$ outside d (see eq. (23)) and hence affect the calculation of moments and transition rates. Specifically, matrix elements $\langle \Phi_k | \mathfrak{g} | \Phi_j \rangle$ are required where $|\Phi_j\rangle$ is in the model space but $|\Phi_k\rangle$ is not. Such matrix elements are given by a perturbation expansion of the form (47); indeed the only change required is that the valence diagrams involved have a number of p - h pairs in the final state in addition to the n entering valence lines.

§ 6. The Reaction Matrix as Effective Interaction

The effective-interaction formalism of § 4 and § 5 connects the properties of complex nuclei with the force between free nucleons. This connection is made within a framework which closely resembles conventional shell-model practice. First, a finite model space d is selected. Second, the expansion (47) is used to derive an effective interaction within d from the force between free nucleons. Third, the resulting eigenvalue problem [eq. (50)] within d is solved to yield the energies of low-lying nuclear states. Recent usage has attached the somewhat inappropriate ⁽¹⁸⁾ adjective 'realistic' to such calculations; thus a realistic shell-model interaction is one derived from the free-nucleon interaction and is to be contrasted with phenomenological interactions which are mere parameterizations of energy-level data. This section and the two following it give an assessment of the present state of the art of shell-model calculation with realistic interactions.

The effective interaction $\mathfrak{g}$ within the model space is given by eq. (47) as the sum of a perturbation expansion in powers of the nucleon-nucleon interaction V . Term-by-term summation of such an expansion is not a useful method of calculation whenever the free-nucleon interaction V contains hard cores (finite or infinite). It is first necessary to resum the infinite subseries of ladder terms whose sum is the Brueckner reaction matrix; ⁽¹⁹⁾ thus hard cores in the nucleon-nucleon interaction are handled by substitution of the reaction matrix G , with finite matrix elements of reasonable size, for the free-nucleon interaction V with large or infinite matrix elements. This leads in the present context to the statement, well-known ⁽²⁰⁾ since the early days of Brueckner theory, that a suitable lowest-order approximation to the effective shell-model interaction is the reaction matrix. This section concerns the reaction matrix as an approximation to the effective interaction $\mathfrak{g}$ defined by eq. (47). The discussion falls into two parts; 1) it is shown that the effective interaction $\mathfrak{g}$ reduces to a reaction matrix in the special case of two nucleons outside a completely inert core,

provided that one-particle excitations from valence to empty orbits can be neglected. ii) A description is given of the results of two-particle shell-model calculations with the reaction matrix as effective interaction.

Consider, then, a nucleus such as O^{18} , Sc^{42} , or Zr^{90} whose mass number is 2 greater than a magic number. The simplest shell-model description of such a nucleus involves two particles outside a closed-shell core, with a model space d spanned by states of the 2-particle configurations $(\tau_1 n_1 \ell_1 j_1, \tau_2 n_2 \ell_2 j_2, \dots)^2$. As basis states $|\Phi_i\rangle$ ($i \in d$) in the 2-particle model space choose $\binom{21}{2}$ the antisymmetrized products or 2-particle determinants

$$|\nu_1 \nu_2\rangle = |\tau_1 n_1 \ell_1 j_1 m_1, \tau_2 n_2 \ell_2 j_2 m_2\rangle \quad (51)$$

where ν denotes a complete set $(\tau n \ell j m)$ of quantum numbers for a single-particle valence state.

Three kinds of single-particle state must be distinguished—occupied or core states, valence states and empty states. Let the core states be labelled by capital letters $A, B, \dots$, the valence states by the letter ν with subscripts, $\nu_1, \nu_2, \dots$ and the empty states by lower-case letters $a, b, \dots$. The core states are often referred to as 'hole' states, the valence and empty states as particle states. The physical situation and the notation are summarized in Fig. 6.

The effective interaction within the 2-particle model space d is given by eq. (47) which now becomes

$$\langle \nu_1 \nu_2 | \mathfrak{H}(E_{\nu}) | \nu'_1 \nu'_2 \rangle = \sum_{p=0}^{\infty} \left\{ \langle \nu_1 \nu_2 | V \left(\frac{Q}{E_{\nu} - \bar{H}_0} V \right)^p | \nu'_1 \nu'_2 \rangle \right\}_{\nu} \quad (52)$$

where Q is the operator which projects out of the model space;

$$Q = \sum_{k \notin d} |\phi_k\rangle \langle \phi_k| \quad (53)$$

and the sum embraces all intermediate states $|\phi_k\rangle$ outside d . The states

$|\phi_k\rangle$ outside d fall into three classes:

1) 2-particle excited states $|\phi_k\rangle_{2p}$ in which both valence nucleons are excited into empty orbits, while the core remains undisturbed;

$$|\phi_k\rangle_{2p} = |ab\rangle. \quad (54)$$

2) 1-particle excited states $|\phi_k\rangle_{1p}$ in which only one valence nucleon is promoted to an empty orbit, while the core remains undisturbed;

$$|\phi_k\rangle_{1p} = |av\rangle. \quad (55)$$

3) States $|\phi_k\rangle_{ce}$ in which the core is excited, with nucleons promoted from core orbits to valence or empty orbits.

Experience with the theory of nuclear matter ⁽²²⁾ suggests that the 2-particle intermediate states $|\phi_k\rangle_{2p}$, whose sum yields the Brueckner reaction matrix, make much the most important contribution to the effective interaction $\mathfrak{g}$. The contributions to $\mathfrak{g}$ of the one-particle intermediate states $|\phi_k\rangle_{1p}$ involve matrix elements of the form $\langle av|V|v_1v_2\rangle$ (see Fig. 7) which vanish identically in nuclear matter because of momentum conservation. Matrix elements which vanish in nuclear matter are expected to be small for finite nuclei; ⁽²³⁾ for this reason shell-model studies with realistic interactions ignore 1-particle intermediate states—usually without comment. ⁽²⁴⁾ Core-excited intermediate states can only be neglected to the extent that the model of an inert core with two valence nucleons is a good physical description of the nucleus under consideration. To put it another way, if the pertinent eigenvectors $|\Psi\rangle$ of the two-particle nucleus under consideration are written in the form [cf. eq. (26)]

$$|\Psi\rangle = \alpha |\Psi_d\rangle + \beta |\Psi_{ce}\rangle + \dots, \quad (56)$$

where $|\Psi_d\rangle$ is the component in d and $|\Psi_{ce}\rangle$ the component in core-excited

configurations bordering on d , (²⁵) then core-excited intermediate states make negligible contributions to $\mathfrak{g}$ only if the quantities $|\beta/a|$, (for finite matrix elements $\langle \Psi_d | V | \Psi_{ce} \rangle$), are vanishingly small. This criterion is never satisfied; thus, as shown in §7, core excitation significantly renormalizes the effective interaction in all two-particle shell-model systems. Nevertheless it is reasonable to neglect core excitation as a first approximation and to correct explicitly for its effects afterwards.

The contributions to $\mathfrak{g}$ of one-particle and core-excited intermediate states will accordingly be ignored. The projection operator Q of eq. (53) reduces to the projector Q_{2p} on to the subspace of unoccupied 2-particle states $|\phi_k\rangle_{2p}$:

$$Q \rightarrow Q_{2p} = \sum_{k(2p)} |\phi_k\rangle_{2p} \langle \phi_k|_{2p} = \sum_{ab} |ab\rangle \langle ab|. \quad (57)$$

(unocc.)

Substitution of Q_{2p} for Q in eq. (52) yields the expansion

$$\begin{aligned} \langle v_1 v_2 | G(E_v) | v'_1 v'_2 \rangle &= \langle v_1 v_2 | V | v'_1 v'_2 \rangle \\ &+ \sum_{ab} \frac{\langle v_1 v_2 | V | ab \rangle \langle ab | V | v'_1 v'_2 \rangle}{E_v - \epsilon_a - \epsilon_b} + \dots \end{aligned} \quad (58)$$

(unocc.)

for the matrix elements of the effective interaction. The change of notation $\mathfrak{g} \rightarrow G$ gives explicit recognition to the fact that eq. (58) is the formal solution, iterated with respect to V , of the equation

$$\begin{aligned} \langle v_1 v_2 | G(E_v) | v'_1 v'_2 \rangle &= \langle v_1 v_2 | V | v'_1 v'_2 \rangle \\ &+ \sum_{ab} \frac{\langle v_1 v_2 | V | ab \rangle \langle ab | G(E_v) | v'_1 v'_2 \rangle}{E_v - \epsilon_a - \epsilon_b} \end{aligned} \quad (59)$$

(unocc.)

characteristic of a Brueckner reaction matrix $G(E_v)$ with starting energy (²⁶) E_v . The diagrammatic form of eqs. (58) and (59) is given

in Fig. 8; G-interactions are represented by wavy lines, V-interactions by dotted lines.

The main formal result of this section has now been established; the effective interaction $\mathcal{V}$ has been shown to reduce to a reaction matrix in the special case of two nucleons outside a completely inert core, provided that one-particle excitation from valence to empty orbits can be neglected.

There have been many two-particle shell-model calculations with realistic interactions. ⁽²⁷⁾ In all of these, of course, the central idea has been to use as effective interaction a reaction matrix computed from a free-nucleon interaction potential. The various calculations differ widely in the techniques used to compute the reaction matrix, in the character of the free-nucleon potentials used and in the degree of accuracy demanded in fitting these free-nucleon potentials to the nucleon-nucleon scattering data. A pattern is now beginning to emerge from these studies; the main qualitative conclusions to be drawn will be discussed here in the context of the special two-particle systems O^{18} and F^{18} .

The model space for O^{18} and F^{18} is the same as that described in § 3 [see eq. (5)] except for the inclusion of $1d_{3/2}$ as an additional valence orbit. Thus the core, valence, and empty orbits are

$$\left. \begin{array}{l} \text{Core orbits: } 1s_{1/2}, 1p_{3/2}, 1p_{1/2} \\ \text{Valence orbits: } 1d_{5/2}, 2s_{1/2}, 1d_{3/2} \\ \text{Empty orbits: } 1f_{7/2}, 2p_{3/2}, \dots \text{ etc.} \end{array} \right\} \quad (60)$$

and the model space d is spanned by states of the configurations $(1d_{5/2}, 2s_{1/2}, 1d_{3/2})^2$. The single-particle energies are taken to have their observed values ⁽²⁸⁾

$$\left. \begin{array}{l} \epsilon(1d_{5/2}) = \epsilon_0 + 0.0 \text{ (MeV)} \\ \epsilon(2s_{1/2}) = \epsilon_0 + 0.87 \\ \epsilon(1d_{3/2}) = \epsilon_0 + 5.08 \end{array} \right\} \quad (61)$$

where $\epsilon_0 = -4.14$ MeV for single-neutron states and $\epsilon_0 = -.60$ MeV for single-proton states. These are the single-particle energies to be used in calculating matrix elements of the effective interaction. In the shell-model matrix diagonalizations, however, ϵ_0 is set equal to zero; ⁽²⁹⁾ in other words, the shell-model energy eigenvalues contain the single-particle energy splittings rather than the true single-particle binding energies to the core.

Consider now two different realistic interactions within d ; both are reaction matrices derived from free-nucleon potentials but they differ widely in the nature of their free-nucleon interactions and consequently in the techniques used to compute their reaction matrices. The first G -matrix is derived from the hard-core interaction of Hamada and Johnston. ⁽³⁰⁾ The second comes from the free-nucleon potential of Tabakin ⁽³¹⁾ which is free of hard cores. It is a sum of separable potentials and provides a reasonably good fit to the S -, P - and D -wave phase parameters up to about 320 MeV.

The Hamada-Johnston reaction matrix was calculated by Kuo ⁽³²⁾ using a refinement of techniques described in an earlier paper by Kuo and Brown. ⁽³³⁾ The starting energy E_v in eq. (59) for G is approximated ⁽³⁴⁾ in a fashion independent of the desired eigenvalue E_v ; specifically, the matrix element $\langle v_1 v_2 | G(\omega) | v_1' v_2' \rangle$ is evaluated with the approximate starting energy

$$\omega = \frac{1}{2} \left\{ [\epsilon(v_1') + \epsilon(v_2')] + [\epsilon(v_1) + \epsilon(v_2)] \right\} \quad (62)$$

The resulting matrix elements of G then define a Hermitian effective Hamiltonian within the model space d . Kuo's method of calculating G will not be discussed here. ⁽³⁵⁾ He uses harmonic-oscillator wave functions for the radial part of the single-particle valence states; no attempt is made to achieve self-consistency in either single-particle energies or single-particle wave functions. ⁽³⁶⁾ The 2-particle intermediate states $|ab\rangle$ in

eq. (59) are approximated by plane waves. ⁽³⁷⁾ Kuo then argues that this plane-wave approximation seriously underestimates the contributions to G of low-lying intermediate states of the special form

$$|ab\rangle = |(1f, 2p)^2\rangle \quad (63)$$

wherein the two valence nucleons are promoted into the lowest available empty orbits, those of the $(1f, 2p)$ shell. He therefore adds such contributions as corrections to the reaction matrix, using second-order perturbation theory. ⁽³⁸⁾ Thus, to follow Kuo's notation, let G be the bare reaction matrix obtained by solution of eq. (59) with the plane-wave approximation in intermediate states and a starting energy ω given by eq. (62); let G_{2p} be the contribution to the reaction matrix of the intermediate states. ⁽⁶³⁾ Then the corrected Hamada-Johnston reaction matrix $\bar{G}$ is taken to be ⁽³⁹⁾

$$\bar{G} = [G + G_{2p}]_{\text{Kuo}} \quad (64)$$

The energy eigenvalues obtained with $\bar{G}$ as effective interaction are then to be compared with those obtained from the Tabakin reaction matrix G_T .

To calculate the Tabakin reaction matrix G_T it is not necessary to solve eq. (59) directly. Since the Tabakin potential is free of hard cores it is sufficient ⁽⁴⁰⁾ to calculate G_T from the first two terms in the perturbation expansion (58). This has been done by Clement and Baranger ⁽⁴¹⁾ who use the approximate starting energy given in eq. (62), with the single-particle energies of eq. (61) and harmonic-oscillator radial wave functions. They find that inclusion of the second-order term in the perturbation expansion has a significant effect on the calculated energy spectra.

The reaction matrices G_T and $\bar{G}$ are now substituted for the effective interaction $\mathfrak{g}$ in eq. (50) and the resulting eigenvalue equations solved for the energy eigenvalues E_v ; since the dependence of the reaction

matrices on E_v has been ignored, solution of this eigenvalue problem reduces to a conventional shell-model calculation within the configurations

$(1d_{5/2}, 2s_{1/2}, 1d_{3/2})^2$. Spectra of O^{18} obtained with G_T and $\bar{G}$ as effective interactions are compared with each other and with experiment ⁽⁴²⁾ in Fig. 9. The experimental energy $\bar{E}$ given in Fig. 9 is

$$\begin{aligned}\bar{E}(O^{18}) &= E^*(O^{18}) - \{B.E.(O^{18}) - B.E.(O^{16}) \\ &\quad - 2[B.E.(O^{17}) - B.E.(O^{16})]\} \\ &= E^*(O^{18}) - 3.91 \text{ MeV.}\end{aligned}\quad (65)$$

where $E^*(O^{18})$ is the excitation energy of the state in question and the necessary ground-state binding energies are taken from the tables of König et al. ⁽⁴³⁾ Spectra of F^{18} are shown in Fig. 10; the experimental energy $\bar{E}$ is

$$\bar{E}(F^{18}) = E^*(F^{18}) - 5.00 \text{ MeV.} \quad (66)$$

The quantity $\bar{E}$ is the interaction energy of the valence nucleons with a small correction from the single-particle energy splittings [eq. (61)]. It is therefore to be compared directly with the energy eigenvalue E_v of the shell-model calculations. ⁽²⁹⁾

Figures 9 and 10 reveal striking agreement between the spectra calculated with the Tabakin reaction matrix G_T and the Hamada-Johnston reaction matrix $\bar{G}$ as effective interactions. Indeed the two sets of calculated spectra agree with each other much more closely than either of them agrees with experiment. The similarity is especially close for O^{18} (Fig. 9) where G_T and $\bar{G}$ lead to almost identical results. Agreement is also close in the case of F^{18} (Fig. 10) although significant differences can now be seen, in particular for the energies of states of spin 2.

It is, of course, possible that the close agreement found between G_T and $\bar{G}$ is fortuitous and that much larger uncertainties in the calculated reaction matrices lie hidden. That this may be the case is

suggested by the fact that there are sizeable differences between the reaction matrices calculated by Kuo and Brown (³³) and those recalculated by Kuo (³²) using what appear to be minor refinements of the original method.

There is, on the other hand, some evidence that the agreement between G_T and $\bar{G}$ may be a fair indicator of the magnitude of the errors and uncertainties involved in the calculation of reaction matrices. First, a similar close agreement between G_T and hard-core reaction matrices has been encountered in studies (⁴⁴) of other $T = 1$ two-particle systems. Second, the fact that errors enter G_T and $\bar{G}$ in basically different ways (⁴⁵) makes accidental agreement less likely. Errors in the Tabakin reaction matrix are probably smaller because the procedure connecting it to the underlying free-nucleon potential is inherently simpler. The weakness in this argument is of course that true differences in the reaction matrices due to differences in the underlying potentials may be masked by errors in calculation. Third, G_T and $\bar{G}$ not only yield very similar 2-particle spectra; it is shown in § 7 that they also yield similar corrections to the spectra for the effects of core excitation. The fact that these corrections systematically improve agreement with experiment suggests that the similarity between G_T and $\bar{G}$ is not entirely accidental.

In the above comparison between G_T and $\bar{G}$ it is impossible to separate the effects of errors in calculating the reaction matrices from true differences due to differences in the underlying potentials. This difficulty is particularly pronounced when the comparison involves qualitatively different free-nucleon interactions such as the smooth Tabakin interaction and the singular Hamada-Johnston interaction. Lynch and Kuo (⁴⁶) have studied the influence on the spectra of O^{18} and F^{18} of the differences between three hard-core free-nucleon interactions; two of these have infinite hard cores, the other a finite core. The reaction matrices are calculated in exactly the same way; thus, since the underlying potentials are qualitatively similar, the errors in calculating the three different reaction

matrices should be of roughly the same size. (⁴⁷) It is found that the three different free-nucleon interactions lead to almost identical spectra in both O^{18} and F^{18} .

It appears, then, that 2-particle shell-model spectra are only moderately sensitive to uncertainties in the reaction matrices. The core energy E_c is a much more sensitive quantity. Reaction matrices which yield very similar 2-particle spectra can lead to very different values of E_c . (⁴⁸) It is likely that many-particle shell-model spectra are also much more sensitive to uncertainties in G (⁴⁹) than are the 2-particle spectra. Thus even if the close agreement between the 2-particle spectra obtained from G_T and $\bar{G}$ is not a mere coincidence but is a true indicator of the uncertainties in G , the study of many-particle shell-model systems (see § 9) will almost certainly demand improved accuracy in the calculation of the reaction matrix.

Return, finally, to Figs. 9 and 10 to assess the quality of agreement between theory and experiment. Since the 2-particle spectra calculated with G_T and $\bar{G}$ as effective interactions are almost identical, the phrase 'calculated spectra' can be applied to one, to the other, or to both without further specification. It is at once clear that the calculated spectra are qualitatively correct; the order and relative spacings of the levels of O^{18} and F^{18} are fairly well reproduced. In O^{18} , however, the calculated spectra are much too compressed (the excitation energies are too small) and there is not nearly enough binding in the calculated O^{18} ground state. These features, incidentally, seem to be characteristic of $T = 1$ two-particle spectra with realistic interactions. (⁵⁰) Overall agreement is better in the case of F^{18} except that the first $1+$ excited state, whose observed excitation energy is 1.7 MeV, appears at above 3 MeV in the calculated spectra. In § 7, these discrepancies between theory and experiment will be discussed in terms of core excitation which was neglected in reducing the effective interaction of eq. (47) to a reaction matrix.

§ 7. Core Excitation in Two-Particle Shell-Model Systems

The effective interaction $\mathfrak{g}$ within the two-particle model space is given in eq. (52) as the sum of a perturbation series that involves the "Pauli operator"

$$\left(\frac{Q}{E_V - \overline{H}_0} \right) = \left(\frac{Q}{e} \right). \quad (67)$$

In § 6 the projection operator Q is expressed as a sum of three parts;

$$Q = Q_{2p} + Q_{1p} + Q_{c.e.} \quad (68)$$

Neglect of the 1-particle term Q_{1p} and the core-excited term $Q_{c.e.}$ (see eqs. (53), (54), (55) and (57)), in other words the approximation

$$\left(\frac{Q}{e} \right) \approx \left(\frac{Q_{2p}}{e} \right), \quad (69)$$

reduces the equation for $\mathfrak{g}$ to a reaction-matrix equation. It is now time to examine the effect of the other terms in eq. (68); specifically, this section concerns a few of the many complicated excitations that contribute to the core-excited projection operator $Q_{c.e.}$

A core-excited state is one in which particles are excited from the occupied orbits of the core to valence or empty orbits. Consider first 3-particle, 1-hole states $[3p, 1h]$ wherein only one core particle is excited (⁵¹); since the valence orbits usually have opposite parity to the highest core orbits, the $(3p, 1h)$ states for which the energy denominators e in eq. (67) are smallest involve the promotion of a core nucleon across two major shells. In harmonic-oscillator parlance, such states are "(3p, 1h) states of excitation energy $2\hbar\omega$." In the case of O^{18} and F^{18} the

pertinent states belong to the configurations

$$\left. \begin{array}{l} (1s)^{-1} (1d, 2s)^3 \\ \text{or} \quad (1p)^{-1} (1d, 2s)^2 (1f, 2p)^1 \end{array} \right\} \quad (70)$$

Introduce the notation

$$Q_0 (3p, 1h) = \sum_{(2\hbar\omega)} |3p, 1h\rangle \langle 3p, 1h| \quad (71)$$

for the projection operator on to the subspace of $(3p, 1h)$ states of excitation energy $2\hbar\omega$. The lowest-order approximation (69) to the Pauli operator will now be replaced by

$$\left(\frac{Q}{e} \right) \approx \left(\frac{Q_{2p}}{e} \right) + \left(\frac{Q_0(3p, 1h)}{e} \right) \quad (72)$$

where the correction for core excitation is to be treated in first-order perturbation theory. Thus when eq. (72) is substituted in the expansion (52) for $\mathfrak{D}$, all terms involving $Q_0(3p, 1h)$ more than once are to be dropped. On the other hand the two-particle term Q_{2p} must be carried to all orders since this is what is involved in the replacement of the free-nucleon interaction V by the reaction matrix G . The expansion (52) becomes, after some rearrangement,

$$\begin{aligned} \mathfrak{D} = & \left\{ V + V \frac{Q_{2p}}{e} V + \dots \right\} \\ & + \left\{ V + V \frac{Q_{2p}}{e} V + \dots \right\} \frac{Q_0(3p, 1h)}{e} \left\{ V + V \frac{Q_{2p}}{e} V + \dots \right\} \end{aligned} \quad (73)$$

Since the terms in curly brackets in eq. (73) are simply G-operators, the approximation to $\mathfrak{g}$ implied by eq. (72) becomes

$$\left. \begin{aligned} \mathfrak{g} &\approx G + \delta\mathfrak{g}_0(3p, 1h) \\ \delta\mathfrak{g}_0(3p, 1h) &= G \left(\frac{Q_0(3p, 1h)}{e} \right) G. \end{aligned} \right\} \quad (74)$$

To illustrate the problems that arise in evaluating matrix elements of $\delta\mathfrak{g}_0$, consider the contributions of states of the configuration $(^{52}) A^{-1}(v)^2a$ to the matrix element $\langle v_1 v_2 | \delta\mathfrak{g}_0 | v'_1 v'_2 \rangle$. Products of the form

$$e^{-1} \langle v_1 v_2 | G | A^{-1}(v^2)a \rangle \langle A^{-1}(v^2)a | G | v'_1 v'_2 \rangle$$

are encountered; these products can be expressed, by standard recoupling techniques $(^{53})$, in terms of products such as

$$e^{-1} \langle v_1 A | G | a v_1' \rangle \langle a v_2' | G | v_2' A \rangle \quad (75)$$

that contain 2-body G-matrix elements. (The intermediate state in the term (75) is $A^{-1}(v_1' v_2')a$).

It is obvious that matrix elements of G are now needed between two-particle states outside the model space. In the studies to be discussed here, all matrix elements of G—inside and outside the model space—are calculated with the approximation to the starting energy described in § 6 (Eq. (62)). The prescription, it will be recalled, is to use as starting energy the average of the single-particle energies on the left- and right-hand sides of the matrix element under consideration. For example, in evaluating the contribution (75) to $\delta\mathfrak{g}_0$, the reaction-matrix element $(^{54}) \langle a v_2' | G(\omega) | v_2' A \rangle$ is to be determined with a starting energy

$$\omega = \frac{1}{2} \left\{ (\epsilon(v_2') - \epsilon(A)) + (\epsilon(a) + \epsilon(v_2)) \right\}. \quad (76)$$

The desired correction term $\delta\vartheta_0(3p, 1h)$ is the sum of all contributions of the sort considered above; all such contributions are generated as the sum in eq. (71) sweeps over all $(3p, 1h)$ states of excitation energy $2\hbar\omega$. Two distinct kinds of contribution emerge. The first, shown in Fig. 11a, is a true correction to a 2-body matrix element of the effective interaction. The second, shown in Fig. 12, is a correction not to a 2-body matrix element but to one of the single-particle valence energies. In taking these single-particle energies from experiment this correction has already been included. Thus care must be taken⁽⁵⁵⁾ to separate the two sorts of contribution to $\delta\vartheta_0(3p, 1h)$ and to ignore the single-particle correction of Fig. 12.

Return now to the reaction-matrix calculations for O^{18} and F^{18} . It will be recalled that Clement and Baranger⁽⁴¹⁾ have computed a reaction matrix G_T from the non-singular free-nucleon potential of Tabakin⁽³¹⁾, while Kuo⁽³²⁾ has evaluated a reaction matrix $\bar{G}$ from the hard-core nucleon-nucleon interaction of Hamada and Johnston⁽³⁰⁾. Both studies proceed to evaluate the core-excitation correction $\delta\vartheta_0(3p, 1h)$ in the manner outlined above. The crude approximation

$$e \approx 2\hbar\omega = 28 \text{ MeV}, \quad (77)$$

is used for the energy denominator in the $(3p, 1h)$ Pauli operator; the $(3p, 1h)$ states under consideration are therefore "states of excitation energy $2\hbar\omega$ " in fact as well as in name.

The calculated spectra of O^{18} and F^{18} , with $(3p, 1h)$ corrections included, are shown in Figs. 13 and 14. The three main points to be noted are as follows;

- 1) The remarkably close agreement between the spectra

obtained with G_T and $\bar{G}$ as effective interactions persists undiminished when (3p, 1h) corrections are added. Again the agreement is particularly striking in O^{18} .

2) (3p, 1h) corrections are small (especially for $T = 0$ states) except for the 0^+ states in O^{18} which are pushed about 1 MeV farther apart. The changes introduced by the (3p, 1h) corrections, although small, are nearly all such as to improve agreement with experiment.

3) The calculated position of the first 1^+ excited state of F^{18} is still more than 2 MeV too high.

All this is perfectly reasonable. The (3p, 1h) corrections are in the right direction but are not so large as to cast doubt on the assumption that they can be treated as a small perturbation. The smallness of (3p, 1h) effects (⁵⁶) is consistent with experience in nuclear shell-model calculations; no indications have been found that the configurations (70) mix strongly in low-lying states of 2-particle shell-model systems.

The situation is quite different for (4p, 2h) corrections. The pertinent intermediate states now belong to the configurations

$$(1p)^{-2} (1d, 2s)^4. \quad (78)$$

These configurations are believed to contribute heavily to low-lying states of O^{18} and F^{18} . For example, Federman and Talmi (⁵⁷) estimate that the two lowest 0^+ states in O^{18} contain admixtures (⁵⁸) of up to 30% of the particular state of the configuration (78) obtained by removing two 1p nucleons from the highly-deformed 0^+ ground state of Ne^{20} . 2^+ states in O^{18} likewise have large components of a state obtained by removing two 1p nucleons from the 2^+ first excited state of Ne^{20} . Such deformed states probably contribute even more strongly (⁵⁹) to low-lying states in F^{18} .

A perturbative treatment of (4p, 2h) corrections to the effective interaction in O^{18} and F^{18} is, accordingly, highly suspect. It would clearly be desirable to extend the model space d to include the configurations (78)—

or at least the physically interesting deformed states to which they give rise—and to recalculate the effective interaction for this new model space. Such a calculation is prohibitively difficult and has not yet been attempted. Kuo (³²) has, however, treated the (4p, 2h) corrections by perturbation theory, with the results shown in Figs. 13 and 14. With both (3p, 1h) and (4p, 2h) (Fig. 11b) corrections, the Hamada-Johnston reaction matrix $\bar{G}$ yields excellent agreement with experiment for the positive-parity spectrum of O^{18} . It also provides a satisfactory account of the energies of all low-lying states of positive parity in F^{18} with the single striking exception of the first 1^+ excited state. This the model places more than 2 MeV above its observed excitation energy of 1.7 MeV.

What, then, are the general conclusions to be drawn? Ignore, for the moment, questions about the applicability of perturbation theory to the calculation of (4p, 2h) corrections and about the striking discrepancy for the first 1^+ excited state in F^{18} ; these matters are discussed in § 8. The strongest impression is that, starting from the force between free nucleons and applying the effective-interaction formalism in reasonably systematic fashion, a detailed fit has been obtained to the energy levels of the 2-particle nuclei O^{18} and F^{18} . Furthermore, this detailed fit has been achieved along two different paths, (⁶⁰) starting from two free-nucleon interactions which fit the scattering data but have little else in common. In spite of the many uncertainties involved, this is a major achievement.

On the other hand, the insensitivity of the level spectra to the detailed properties of the free-nucleon interaction has its disappointing aspects. The indications are that any force that provides a reasonable fit to the scattering data leads to much the same level spectra. This suggests that the study of level energies in complex nuclei will not provide much additional information about the forces between free nucleons.

§ 8. Deformed States and State-Dependence of the Effective Interaction in O^{18} and F^{18} .

Two points were left in the air at the end of § 7; doubt was expressed about the applicability of perturbation theory to (4p, 2h) corrections and a striking discrepancy amidst otherwise excellent agreement with experiment was noted for the lowest 1^+ excited state of F^{18} .

Both these points are closely connected with the existence of sizeable deformed components in the wave functions of low-lying states of O^{18} and F^{18} . Deformed intrinsic states in O^{18} and F^{18} are made ⁽⁶¹⁾ by removing two nucleons in the highest 1p-shell Nilsson orbit from the deformed intrinsic ground state of Ne^{20} . The deformed (4p, 2h) shell-model states under consideration are simply the angular-momentum eigenstates projected from this deformed intrinsic state. The deformed states so obtained have spins 0^+ , 2^+ and 4^+ in O^{18} , 1^+ , 3^+ and 5^+ in F^{18} .

Now the quantitative importance of a deformed state depends critically on its unperturbed position. This can be estimated in various ways—from the measured binding energies of states of similar structure in neighboring nuclei, ⁽⁵⁷⁾ by direct calculation with an assumed shell-model interaction ⁽⁶²⁾ or with the help of an approximate formula due to Zamick. ⁽⁶³⁾ There are large uncertainties; the unperturbed positions of the lowest deformed states are not well determined. The indications are, however, that the lowest deformed states in O^{18} occur between 4 and 5 MeV above the ground state; states below 4 MeV in O^{18} then contain up to 30% admixtures ⁽⁵⁸⁾ of deformed states. Binding-energy considerations ⁽⁶⁴⁾ indicate that the lowest deformed state in F^{18} has spin 1^+ and occurs less than 1.5 MeV above the ground state. ⁽⁶⁵⁾

Now the O^{18} levels treated in § 6 and § 7 within the 2-particle model space all ⁽⁶⁶⁾ lie below 4 MeV; thus the lowest deformed excitations are about 1 MeV above the states of the model. Deformed (4p, 2h) admixtures in these model states are 30% or less in intensity. In this situation a perturbative treatment of corrections to the effective interaction is marginal but not obviously incorrect.

The situation is quite different in F^{18} . The lowest deformed state occurs between 1 and 2 MeV above the ground state, in the midst of the states that the model seeks to describe. There are three levels below this lowest deformed state—the 1^+ ground state, the 3^+ first excited state and the 5^+ second excited state. These states probably have deformed components of similar size to those in the low-lying states of O^{18} ; the treatment of (4p, 2h) corrections by perturbation theory is again doubtful but not clearly incorrect. For all higher states, however, a perturbative treatment of (4p, 2h) corrections is out of the question. In particular, the 1^+ state at 1.7 MeV in F^{18} is probably dominated by its (4p, 2h) deformed component; to describe such a state within the 2-particle model space with only a perturbative treatment of its dominant component is manifestly wrong.

Thus, with the above model space and effective interaction, a comparison of theory and experiment for level-energies in F^{18} is significant only for the three lowest levels. In particular, the large discrepancy between the calculated and observed energies of the 1^+ excited state at 1.7 MeV simply reflects the fact that the model state and the observed level have little in common.

More is involved here than a mere breakdown of lowest-order perturbation theory. It will be recalled from the discussion at the end of § 4 that a strongly state-dependent (i. e. E-dependent) effective interaction can be expected whenever, in the midst of energy levels to be treated within a model space d , there lies a highly collective state arising predominantly from higher configurations. This is precisely the situation here. It is accordingly unlikely that there is any single effective interaction within the 2-particle model space that gives a satisfactory description of both the 1^+ ground state and the 1^+ excited state at 1.7 MeV. Rather than concoct a state-dependent interaction, it is probably better to extend the model space to include the (4p, 2h) deformed states that strongly influence the low-lying spectra. This extended calculation is also necessary to decide

whether or not a perturbative treatment is valid for (4p, 2h) corrections in states with relatively small deformed components; it is impossible to establish the accuracy of an approximation by invoking agreement with experiment.

§ 9. The Many-Particle Shell Model

The extension of the formalism of §§ 4, 5 and 6 to accommodate valence holes as well as valence particles is straightforward. ⁽⁶⁾ So far only 1p-1h systems have been studied quantitatively. ⁽⁶⁷⁾ Once again the leading term in the effective interaction is a reaction matrix, which now enters through its hole-particle matrix elements. ⁽⁶⁸⁾ de Takacsy ⁽⁶⁹⁾ has enumerated the lowest-order core-excitation diagrams in 1p-1h systems and has estimated them for negative-parity states in O^{16} using a Rosenfeld interaction as a substitute for the bare G-matrix. He finds that the main correction terms tend to cancel so that core excitation renormalizes G very much less than it does in 2-particle systems.

Consider next the many-particle shell model, with n valence particles ($n > 2$). The matrix elements of the effective interaction $\mathfrak{g}$ between n -particle model states are given by the perturbation expansion (47). Start as in the 2-particle system by dropping all intermediate states $|\phi_k\rangle$ in the projection operator Q except those in which 2 valence nucleons are excited into empty orbits. Furthermore, in iterating this reduced two-particle projection operator, keep only those terms in which it is always the same two valence nucleons that are excited. The sum of all such terms is the matrix element between n -particle states of the two-body G-operator for the 2-particle system whose valence orbits are the same as those of the n -particle system under consideration. The resulting approximation to the n -particle effective interaction is thus the appropriate 2-particle reaction matrix. The lowest-order effective interaction is given in the case $n = 3$ by the type of diagram shown in Fig. 15a). The necessary matrix elements of $\mathfrak{g}$ between

n-particle model states are computed in terms of the 2-body matrix elements of G by standard shell-model techniques.

As in the two-particle system, it will usually be necessary to consider core excitation. To do this treat in lowest -order perturbation theory selected core-excited intermediate states $|\phi_k\rangle_{c.e.}$ in the projection operator Q of eq. (47). In iterating, retain only those terms in which interactions are attached to no more than two of the n valence lines. Some of the resulting diagrams yield corrections to the single-particle valence energies. The others are core-excitation modifications of the bare 2-particle reaction matrix. For example, to obtain the diagrams representing the changes in the n -particle effective interaction due to perturbative (3p, 1h) and (4p, 2h) corrections to the 2-particle reaction matrix, simply add $n-2$ passive valence lines to Figs. 11a and 11b. Such corrections are included by replacing the 2-body matrix elements of G by corrected two-body matrix elements and computing the matrix elements between n -particle states as before.

All the terms so far considered give 2-body contributions to the n -particle effective interaction $\mathcal{G}$. Many-body terms are introduced by dropping the restriction that, in iterating the projection operator Q in eq. (47), only those terms are to be kept in which interactions are attached to no more than two valence lines. A 3-body term for $n = 3$ is shown in Fig. 15 b).

Consider next 3-body diagrams that do not involve core excitation. Such terms are obtained by replacing Q in eq. (47) by the 2-particle projection operator Q_{2p} of eq. (57) and selecting 3-body contributions. Some diagrams of this sort for $n = 3$ are shown in Fig. 16. The sum of all such diagrams can be obtained, following Bethe⁽⁷⁰⁾ and Day⁽⁷¹⁾, by solving a Faddeev equation⁽⁷²⁾ which is the 3-body generalization of the equation for the 2-body reaction matrix.

It is clear that an appropriately corrected 2-particle G -matrix will give the dominant contribution to the n -particle effective interaction $\mathcal{G}$. Many-body contributions should be relatively small. In order

to study such effects in many-particle spectra it will be necessary to achieve greater accuracy in the calculation of the reaction matrix and its core-excitation corrections; in the present state of the art uncertainties in G might well swamp the many-body effects under consideration.

To conclude, shell-model calculations with realistic interactions have been carried out only for 2-particle systems and for 1p-1h systems. The calculation of the effects of core excitation in such systems is still at an early stage of its development. Many-particle systems have not been studied at all.⁽⁷³⁾

§ 10. Phenomenological Shell-Model Interactions

Shell-model calculations with realistic interactions have so far been carried out only for 2-particle and for 1p-1h systems. Many-particle shell-model studies continue to rely on a phenomenological procedure wherein the effective interaction $\mathfrak{V}$ is parameterized in some simple fashion and the parameters are determined by direct comparison with experiment. This phenomenological procedure will now be described, illustrated in an application to O^{18} and F^{18} and, finally, compared and contrasted with the procedure developed in §§ 4—9, where effective interactions are derived from the forces between free nucleons. A complete title for this section would therefore be "Phenomenological Shell-Model Interactions and their Relation to Realistic Interactions."

It is assumed from the outset that the many-particle effective interaction $\mathfrak{V}$ reduces to a two-body interaction $\mathfrak{V}_2$. Within the finite model space of the many-particle configurations $(j_1, j_2, \dots, j_\mu)^n$ this two-body operator is completely determined by a finite set of numbers, its matrix elements ⁽⁷⁴⁾

$$\langle j_1 j_2^{JT} | \mathfrak{V}_2 | j_3 j_4^{JT} \rangle \quad (79)$$

between the possible antisymmetric two-particle states of the configurations under consideration. Since the two-body matrix elements constitute a finite set they can themselves be treated as independent parameters to be evaluated by a least-squares fit to observed level-energies. ⁽⁷⁵⁾

To illustrate this procedure return once more to the nuclei O^{18} and F^{18} . Choose the restricted model space described in § 3 (eq. 5); the O^{16} core is assumed to be inert and the two valence particles populate the $1d_{5/2}$ and $2s_{1/2}$ orbits. The effective two-body interaction $\mathfrak{V}_2$ in the model space of the configurations $(1d_{5/2}, 2s_{1/2})^2$ is then characterized by its 16 two-body matrix elements — 8 in states with $T = 0$ (F^{18}), 8 in states with $T = 1$ (O^{18}).

The two-body matrix elements cannot be determined from the 2-particle spectra alone ⁽⁷⁶⁾; the configurations $(1d_{5/2}, 2s_{1/2})^2$ contain only 12 states and there are 16 matrix elements to be determined. Information about the many-particle configurations $(1d_{5/2}, 2s_{1/2})^n$ must therefore be introduced. It is here, of course, that the assumption that $\mathfrak{V}$ is a two-body operator assumes critical importance.

Consider therefore the nuclei O^{18} , F^{18} , O^{19} , F^{19} , O^{20} , F^{20} and Ne^{20} . They are to be described within the configurations $(1d_{5/2}, 2s_{1/2})^n$. The single-particle energies (eq. (61) with $\epsilon_0 = 0.0$ MeV) and the two-body interaction $\mathfrak{V}_2$ are assumed to be the same in all the nuclei under consideration. The 16 two-body matrix elements of $\mathfrak{V}_2$ are determined by a least-squares fit to the energies of the following 36 levels of well-determined spin and positive parity;

O^{18} : g. s. (0), 1.98(2), 3.55(4), 3.63(0), 3.92(2), 5.37(3)

F^{18} : g. s. (1), 0.94(3), 1.13(5), 2.53(2)

O^{19} : g. s. ($\frac{5}{2}$), 0.10($\frac{3}{2}$), 1.47($\frac{1}{2}$), 2.78($\frac{3}{2}$), 3.15($\frac{5}{2}$)

F^{19} : g. s. ($\frac{1}{2}$), 0.20($\frac{5}{2}$), 1.56($\frac{3}{2}$), 2.79($\frac{9}{2}$)

O^{20} : g. s. (0), 1.67(2), 3.57(4), 4.07(2), 4.45(0)

F^{20} : g. s. (2), 0.65(3), 1.06(1)

Ne^{20} : g. s. (0), 1.63(2), 4.25(4), 6.75(0), 7.46(2), 8.60(0), 8.79(6),
9.11(4), 11.99(8).

The excitation energy of each state is given in MeV. with its spin in brackets. Note that the 1^+ state at 1.7 MeV in F^{18} is not included in the above list; it is omitted because, as discussed in § 7, its dominant components probably lie outside the 2-particle model space. The effect of including this state in the fitting procedure is described in § 11.

The two-body matrix elements x_r ($r = 1$ to 16) are therefore varied until a local minimum (⁷⁷) is found for the function

$$\chi^2 = \sum_{k=1}^{36} \left[E_k^{\text{exp}} - E_k^{\text{calc.}}(x_r) \right]^2 \quad (80)$$

where E_k^{exp} is the observed (⁷⁸) energy of state k and $E_k^{\text{calc.}}(x_r)$ is the energy obtained from a shell-model calculation with the two-body matrix elements $\{x_r\}$. The sum over k embraces the 36 states listed above, (⁷⁹) E_k^{exp} is an excitation energy if k is an excited state; if it is a ground state

$$E_k^{\text{exp}} = - \{ \text{B. E.}(N, Z) - \text{B. E.}(O^{16}) - 4.14(N-8) - 0.60(Z-8) \} \quad (81)$$

where N and Z are the nucleon-numbers of the nucleus in question and all energies are in MeV, (cf. eqs. (65) and (66)). The values $\{x_r^0\}$ of the two-body matrix elements at minimum determine the best-fit two-body interaction $\mathfrak{V}_2$; the corresponding model energies $E_k^{\text{calc.}}(x_r^0)$ give the best fit (in the least-squares sense) to the observed level spectra that can be achieved within the chosen configurations $(1d_{5/2}, 2s_{1/2})^n$.

The quality of the resulting best fit (⁸⁰) can be inferred from Tables 1 and 2 and from Figs. 17 and 18. The model describes the spectra of the isotopes of O, F and Ne with fair accuracy; only a few salient features of this comparison between theory and experiment will be mentioned here.

The calculated and observed levels of F^{19} are compared in Table 1. F^{19} has four positive-parity states up to 2.79 MeV followed by a 1 MeV gap before the next positive-parity state (whose spin is unknown) at 3.915 MeV. The four low-lying states, their spin sequence and the subsequent 1 MeV gap are satisfactorily reproduced by the model.

Table 2 gives the energies of positive-parity levels in Ne^{20} . The rotational energy-structure of this nucleus is reproduced with remarkable accuracy by the truncated shell model. Furthermore, the Ne^{20} fit imposes few constraints on the interaction parameters not already implied by fitting the spectra of O and F. The least-squares fit was in fact repeated⁽⁸⁰⁾ with a 30-level least-squares function that includes only the ground state, the 6.75 MeV 0^+ state and the 8^+ state at 11.99 MeV, of the nine Ne^{20} levels listed above. The resulting effective interaction and energy spectra (including that of Ne^{20}) are almost identical to those obtained with all nine Ne^{20} levels in the fit.

The calculated spectra of O^{18} and F^{18} are compared with experiment in Figs 17 and 18. The quality of agreement between theory and experiment is about the same as or a little better than that obtained in § 7 within the configurations $(1d_{5/2}, 2s_{1/2}, 1d_{3/2})^2$ with a realistic interaction including (3p, 1h) and (4p, 2h) corrections. The phenomenological interaction $\mathfrak{J}_2$ has thus been able to absorb the effects of the $1d_{3/2}$ orbit as well as those of core excitation. The 1^+ level at 1.7 MeV in F^{18} appears from Fig. 18 to have no model counterpart; the lowest 1^+ excited state (the only one) in the model occurs at 8.75 MeV.

Phenomenological effective interactions $\mathfrak{J}_P$ are determined by the least-squares fitting procedure just described. Realistic interactions $\mathfrak{J}_R$ are calculated from the free-nucleon interaction by the methods presented in §§ 4—9. The two procedures differ in a number of significant ways; $\mathfrak{J}_P$ and $\mathfrak{J}_R$ are in fact defined differently. 1) The realistic interaction $\mathfrak{J}_R$ is given by equations (eq. (47)) derived on the assumption that the model

eigenvector $|\psi_d\rangle$ is the projection of the true eigenvector $|\psi\rangle$ on the model space d . The least-squares fitting procedure that leads to $\mathfrak{V}_P$ places no restriction whatsoever on the model eigenvector $|\psi_d\rangle$. 2) The phenomenological interaction $\mathfrak{V}_P$ is assumed from the outset to be a Hermitian two-body operator; $\mathfrak{V}_R$ is only approximately Hermitian and contains many-body terms. 3) $\mathfrak{V}_P$ is determined by a simultaneous fit to the spectra of several different nuclei. In order to obtain enough data to fix the two-body matrix elements, it is often necessary to include in the fit nuclei whose mass numbers differ by as much as 10 to 20. Thus $\mathfrak{V}_P$ includes all sorts of complicated effects — corrections to the valence single-particle energies, core excitation, many-body effects — in a totally inextricable fashion. The realistic interaction $\mathfrak{V}_R$ treats one nucleus at a time and exhibits clearly and separately the various different physical effects that it contains.

Some of the implications of these differences in the defining procedures of $\mathfrak{V}_P$ and $\mathfrak{V}_R$ will be discussed in § 11 and § 12. The quantitative differences are probably quite small — particularly the many-body corrections and the effects of the non-Hermiticity of $\mathfrak{V}_R$. Nevertheless $\mathfrak{V}_P$ and $\mathfrak{V}_R$ are the answers to different questions. It does not make much sense to compare tables of phenomenological and realistic matrix elements for the same choice of configurations. Realistic shell-model interactions can and should be assessed by comparing their predictions directly with experiment.

§11. Phenomenological Study of Deformed States in O^{18} and F^{18} — the Anatomy of a Forced Fit.

(4p, 2h) corrections to the effective interaction were discussed within the reaction-matrix formalism in §§8 and 9. The main corrections of this sort for low-lying states of O^{18} and F^{18} stem from deformed states of the (4p, 2h) configurations $1p^{-2}(1d, 2s)^4$. The order of magnitude and the qualitative properties of these (4p, 2h) corrections are found to be consistent with what is known about deformed states in O^{18} and F^{18} . Thus the shell model with realistic interactions not only fits the energies of nuclear states but also yields information about their configuration structure.

Can such information also be extracted from the phenomenological fits presented in §10? The main difficulty in doing so is that physically distinct contributions to the phenomenological interaction cannot be distinguished from each other and exhibited for individual scrutiny. The best that can be done is to study the influence of various levels of interest on the quality and character of the least-squares fit. The idea is to hunt for forced fits. If the mere presence or absence in the fitting procedure of a single level or of a few related levels has a critical influence on the quality of the fit to the remaining data, it is likely that the model is being forced to accommodate states whose configuration structure does not suit its requirements.

Consider first the influence of the 0^+ state at 3.63 MeV in O^{18} — one of the states which, according to the discussion in §8, have deformed components of about 30% in intensity. Omit this 0^+ state from the 36-level least-squares function of eq. (80). Omit also the $\frac{5}{2}^+$ state at 3.15 MeV in O^{19} and the 0^+ state at 4.45 MeV in O^{20} since these levels have strong parentage relations with the excited 0^+ state of O^{18} . The resulting 33-level fit⁽⁸⁰⁾ is almost identical to the original 36-level fit; the effective interaction is not significantly altered. The model now predicts the existence of a 0^+ state at 3.72 MeV in O^{18} , a $\frac{5}{2}^+$ state at 3.23 MeV in O^{19} and a 0^+ state at 4.53 MeV in O^{18} — in each case within 100 keV of the appropriate observed level.

Even when they are not included in the fitting procedure the energies of these moderately deformed states are fitted to within 100 keV. The situation for the 1^+ state at 1.7 MeV in F^{18} is quite different. Its energy is not included in the fitting procedure described in §10; the model then predicts an excitation energy of 8.75 MeV for the first excited 1^+ state in F^{18} . This spectacular discrepancy, of course, confirms the conclusion reached in §8 that the 1^+ state at 1.7 MeV in F^{18} belongs predominantly to configurations outside the 2-particle model space.

There can be no doubt that a state has been found that is not appropriate for inclusion in the 2-particle model space. An excellent opportunity is therefore at hand for a study of the anatomy of a forced fit. What happens when the 1^+ state at 1.7 MeV in F^{18} is added to the 36-level fit described in §10? The result⁽⁸⁰⁾ is a description of the isotopes of O, F and Ne that is markedly different in character and, for the 36 states in the original fit, much poorer in quality. First, there are large changes in the two-body matrix elements of the effective interaction; some of the largest changes are

$$\begin{aligned}
 \langle \frac{5}{2} \frac{5}{2} 10 \mid \mathfrak{g}_2 \mid \frac{5}{2} \frac{5}{2} 10 \rangle &: 0.01 \rightarrow -4.33 \\
 \langle \frac{5}{2} \frac{5}{2} 10 \mid \mathfrak{g}_2 \mid \frac{1}{2} \frac{1}{2} 10 \rangle &: -4.27 \rightarrow -0.89 \\
 \langle \frac{5}{2} \frac{5}{2} 01 \mid \mathfrak{g}_2 \mid \frac{1}{2} \frac{1}{2} 01 \rangle &: -1.04 \rightarrow -1.61 \\
 \langle \frac{5}{2} \frac{1}{2} 20 \mid \mathfrak{g}_2 \mid \frac{5}{2} \frac{1}{2} 20 \rangle &: -3.70 \rightarrow -2.87
 \end{aligned} \tag{82}$$

where the notation for the matrix elements is given by the expression (79) and all matrix elements are in MeV. The average change in the twelve remaining matrix elements is 400 keV. Moreover, this large change in the effective interaction produces correspondingly large changes in the calculated spectra. The first excited 1^+ state in F^{18} is, of course, greatly lowered in energy; it now appears at 2.34 MeV. The quality of agreement between theory and experiment for the other 36 states deteriorates uniformly. F^{18} acquires a model ground-state spin of 3^+ . The $\frac{3}{2}^+$ second excited state of F^{19} , whose observed

excitation energy is 1.56 MeV, appears at 2.48 MeV. The general deterioration is illustrated in Table 3, which lists the calculated level-energies in O^{19} .

Inclusion of the 1^+ state at 1.7 MeV in F^{18} in the fitting procedure therefore reveals two characteristic features of a forced fit. The first is the pathological fashion in which one state out of 37 critically influences the quality of the fit to the energies of the remaining 36. The second is the generally poor quality of agreement between theory and experiment.

The argument has, in a sense, proceeded backwards. It had already been concluded from other considerations that the F^{18} state at 1.7 MeV differs significantly from its neighbors⁽⁸¹⁾ in configuration structure. This led directly to a study of the influence on the fit of a known intruder. Can the argument be reversed and the fact that the 1^+ state at 1.7 MeV in F^{18} is an intruder inferred from an examination of the fit itself?

Suppose, then, that the results of the 37-parameter fit described above are available and that there are no other clues⁽⁸²⁾ to the configuration structure of the states involved. An obvious procedure is to test what happens when the states with the largest errors in their calculated excitation energies are eliminated, in order of decreasing error, from the fitting procedure. Most of the states singled out in this fashion will be found to have little influence on the character and quality of the fit. Eventually, however, the intruders should be uncovered.

This procedure works quite well in the 37-level fit under consideration; here the three states with the largest errors in their calculated excitation energies are the 1^+ state at 1.06 MeV in F^{20} , the $\frac{3}{2}^+$ state at 1.56 MeV in F^{19} and the 1^+ state at 1.70 MeV in F^{18} . Elimination of the first two states does not have a large effect on the fit; their large errors are probably due to the fact that d_3 admixtures in the $F^{19} \frac{3}{2}^+$ state and in low-lying states of F^{20} are much larger⁽⁸³⁾ than they are in the O isotopes and in F^{18} . Elimination of the third state has been shown to alter the fit radically both in character and in quality; the fact that the configuration structure of the 1^+ state at 1.70 MeV in F^{18} does not

lend itself to a fit within the 2-particle model space has been discovered by examination of the fit itself.

In real physical situations, of course, information from other sources is usually available to guide the search for misfits in phenomenological shell-model calculations. Data on moments, transition rates and reaction cross sections are of great importance here, in addition to qualitative considerations of the kind exemplified in the discussion of deformed states in §8. It will often be possible to go beyond a mere identification of misfits and to say something about the nature of their excited configurations.

To summarize, phenomenological shell-model calculations confirm the conclusions, reached in §8 on the basis of shell-model studies with realistic interactions, ⁽⁸⁴⁾ about deformed (4p, 2h) components in the states of O^{18} and F^{18} . Deformed admixtures in the states of O^{18} and in the three lowest states of F^{18} seem to be of moderate size—no more than 30% in intensity. Such configuration impurities are easily absorbed by the phenomenological effective interaction and are successfully (but possibly not validly) included in the realistic interaction by lowest-order perturbation theory. On the other hand, the 1^+ state at 1.7 MeV in F^{18} cannot be accommodated within the two-particle model space. The difficulty here is not simply that the 1^+ state in question has a large core-excited exponent. That the shell model with effective interaction can absorb huge amounts of configuration impurity is clear from the "pseudonium" studies of Cohen, Lawson and Soper. ⁽⁸⁵⁾ The point seems to be that the pertinent 1^+ state in F^{18} has a much larger core-excited component than its immediate neighbors. This, it will be recalled, is the situation discussed at the end of §4 as a likely source of strong state-dependence in the effective interaction.

Thus the phenomenological shell model and the shell model with realistic interactions lead to similar conclusions about the configuration structure of states in O^{18} and F^{18} . Characteristically, the information yielded by the phenomenological shell model is less specific and is buried more deeply in a surrounding soil of irrelevant numbers.

§12. Moments and Transition Rates

So far in these lectures much has been said about the calculation of level energies and nothing about moments and transition rates. The brief discussion in this section will fall far short of restoring balance. However, imbalance in this connection is not an unmitigated misfortune since it accurately reflects the present situation in nuclear shell theory. Shell-model calculations, both phenomenological and in the reaction-matrix formalism, deal with moments and transition rates much more primitively than energies.

Given⁸⁶ the operator T that determines the rate of a certain transition between nuclear states $|\Psi\rangle$ and $|\Psi'\rangle$, its matrix elements must be calculated within the finite model space d . Thus if $|\Psi_d\rangle$ and $|\Psi'_d\rangle$ are the model states corresponding to $|\Psi\rangle$ and $|\Psi'\rangle$, an effective operator T_{eff} must be found such that

$$\langle \Psi_d | T_{\text{eff}} | \Psi'_d \rangle = \frac{\langle \Psi | T | \Psi' \rangle}{\sqrt{\langle \Psi | \Psi \rangle \langle \Psi' | \Psi' \rangle}} \quad (83)$$

(Recall that the model states are normalized to unity [eq. (25)] but the original eigenvectors $|\Psi\rangle$, $|\Psi'\rangle$ are not.)

In the formalism of §§4-6 —the reaction-matrix formalism—the model states are the projections of the true eigenvectors on the model space d . The basic equations (23) and (24) then determine the true eigenvectors completely; components within d are given as solutions of an eigenvalue problem, components outside d are given directly in terms of the components inside d by eq. (23). Thus in principle all that is needed to calculate T_{eff} is already available. It is, of course, a complicated task to convert this rough scheme into a practical procedure for the calculation of transition-matrix elements. The main difficulty is the one discussed in §5 for energies—the separation of core and valence contributions. The reduction must be achieved both for the matrix elements of T and for the normalization factors. Brandow⁶ has solved this problem for an arbitrary

one-body operator T ; matrix elements within d of the appropriate effective operator are given by a linked perturbation expansion.

This formalism has been applied to the calculation of nuclear moments and transition rates only in the limiting case that the defect wave functions $|\Psi - \Psi_d\rangle$ and $|\Psi'' - \Psi'_d\rangle$ are small perturbations. The linked-cluster formalism is then unnecessary. Noya, Arima and Horie⁽⁸⁷⁾ have computed such corrections to the magnetic-moment operator with a delta-function effective interaction. Mavromatis, Zamick and Brown⁽⁸⁸⁾ have extended these calculations to second order in the defect wave functions using as effective interaction a reaction matrix computed by Kallio and Kolltveit⁽²⁷⁾ from a schematic⁽⁸⁹⁾ hard-core force. It is found that perturbative corrections to magnetic moments are large, that second-order effects are often significant and that the corrections usually improve agreement with experiment.

Consider now the phenomenological shell model. The least-squares fitting procedure that determines the effective interaction places no restriction on the model states $|\Psi_d\rangle$; it yields no information about the relation between the transition operators T and T_{eff} of eq. (83). The only possible way to treat transitions is therefore to parameterize T_{eff} in the same way as the effective interaction. Let T , then, be a one-body operator of multipolarity k . Assume⁽⁹⁰⁾ that T_{eff} is a one-body operator; its multipolarity is of necessity k . T_{eff} is thus completely determined within the model space by a finite set of numbers, its one-body matrix elements

$$\langle j || T_{\text{eff}}^k || j' \rangle ;$$

j and j' are single-particle valence orbits and the matrix elements are reduced in the sense of the Wigner-Eckart theorem.⁽⁹¹⁾ The one-body matrix elements are now to be determined by a least-squares fit to observed moments and transition rates, using the model states $|\Psi_d\rangle$ corresponding to the best-fit effective interaction.

This procedure has never been carried out in detail, probably because it would yield relatively little information of physical interest to repay the effort involved. Calculations of the kind under consideration are, however, carried out in a very restricted fashion in studies of E2 transition rates and magnetic moments. In such studies T_{eff} is assumed to be identical in form to T ; however, the free-nucleon charges and gyromagnetic ratios in T are replaced by effective values. These effective-charge calculations⁽⁸⁶⁾ work well enough to suggest that T_{eff} for E2 and M1 transitions is, in fact, quite similar in structure to T .

Shell-model calculations of moments and transition rates usually proceed on the assumption that

$$T_{\text{eff}} \approx T; \quad (84)$$

it is assumed that truncation has no effect on the transition operator. This cannot be a good approximation since many situations are known in which transition rates and moments are acutely sensitive to configuration impurities. Nevertheless, the shell model with unmodified transition operators provides a remarkably useful framework for the discussion of moments and transition rates; indeed, it sometimes yields detailed agreement with experiment.⁽⁹²⁾ To shed light on this apparent contradiction, note that, whatever their differences in other respects, T and T_{eff} have in common their multipolarity and their one-body character. It is then a reasonable inference that these common features must be responsible for most of the success of the shell model in dealing with transition rates. In other words, the rates of transitions between low-lying nuclear states are determined predominantly by angular-momentum selection rules (including ℓ -selection rules) and by other selection rules (such as those involving seniority) that depend only on the one-body character of the transition operators.

The above discussion compares and contrasts two different procedures for shell-model calculations of moments and transition rates. The first is that of the reaction-matrix formalism, the second is the

phenomenological procedure. Each has been applied in detail only in the lowest approximation. Prospects are brighter for a more detailed study of nuclear transition rates within the reaction-matrix framework since there the different physical effects contained in the effective transition operators are exhibited explicitly.

§13. Future Prospects for Nuclear Shell Theory

The shell model, like the Roman god Janus, has two faces that look in opposite directions. One face looks towards the free-nucleon scattering data, the other towards the spectra of complex nuclei. In other words, the shell model is both a theoretical framework and a phenomenological model. The aim of nuclear shell theory is to unite these two aspects of its personality into a single conceptual structure, within which it is possible to calculate the level properties of complex nuclei in terms of the forces between free nucleons.

The reaction-matrix formalism described in §§4-9 is an attempt to achieve such a unification of nuclear shell theory. It has already had a considerable degree of success. (See §§7-9.) Yet the task of unification is far from complete; serious conceptual difficulties remain and the range of applications has been very narrow.

The main conceptual difficulty is that described in §4—the state dependence of the effective interaction. The point here is that since the model eigenvectors are the projections of the true eigenvectors on the model space, they are not, in general, orthogonal. Thus there cannot be a Hermitian effective Hamiltonian within the model space. This manifests itself in the equations for the effective interaction [eq. (24)] as a dependence of the interaction operator on the eigenvalue E . Thus in principle there is a different effective interaction for every model eigenstate. In order to produce a shell-model eigenvalue problem of the standard kind this state dependence must be ignored. Situations of physical interest in which state-dependent effects may be sizeable are described in §4 and §8. There have, however, been no systematic studies of the state (E)-dependence of the shell-model effective interaction.

In §§6 and 7, where the reaction-matrix formalism is applied to the spectra of O^{18} and F^{18} , the hard-core free-nucleon interaction of Hamada and Johnston⁽³⁰⁾ and the soft-core interaction of Tabakin⁽³¹⁾ are discussed on the same footing. The only visible difference is in the method of calculating reaction matrices. Points of difference⁽⁹³⁾ between the treatments of the two kinds of interaction and questions as to their relative desirability on physical grounds are not discussed. Such matters do not directly effect the main topic of these lectures—the influence of truncation on the nucleon-nucleon interaction. The discussion of truncation effects proceeds in the same way whether the lowest-order approximation to the effective interaction is the unmodified⁽⁹⁴⁾ V operator of a smooth interaction or the reaction matrix of a hard-core interaction.⁽⁹⁵⁾

It was stated above that the range of applications of the reaction-matrix formalism has been very narrow. In fact, only 2-particle and 1p-1h systems have been studied in detail. In addition to all the problems that arise for 2-particle systems, many-particle systems involve new effects and new complications. There are possible many-body contributions to the effective interaction, corrections to the core energy due to the filling of the valence orbits and corrections to the valence single-particle energies. Furthermore it is clear that the degree of accuracy achieved in calculating reaction matrices, although adequate for the treatment of 2-particle spectra, will have to be improved for quantitative studies of many-particle spectra.⁽⁹⁶⁾

Consider next the treatment of configurations bordering on the model space. If admixtures from neighboring configurations are small their effects can be estimated by perturbation theory; if they are large, an extension of the model space is unavoidable. Studies of 2-particle spectra suggest that with model spaces of conventional size (3 or 4 particles in 3 or 4 active orbits) the latter situation is the rule rather than the exception. A clear example was encountered in §8. Deformed (4p, 2h) components in the low-lying states of F^{18} —particularly the 1^+ state at 1.7 MeV—are

certainly large enough to demand, for a proper treatment of the spectrum, extension of the model space from the 2-particle configurations $(1d, 2s)^2$ to include many-particle configurations $1p^{-2}(1d, 2s)^4$. Even in F^{18} , a light nucleus involving orbits of low spin, the resulting extended shell-model calculations lie at the very outer margin of possibility. Anything significantly larger would baffle available computing techniques. What, then, is the prospect for many-particle calculations in heavier nuclei? Can shell-model calculations be carried out in sufficiently extended model spaces to allow a perturbative treatment of the effects of neighboring configurations?

It is certain that the answer to this question is "no" if the pertinent shell-model calculations are to involve construction and diagonalization of the complete energy matrices in the model configurations. The insurmountable problem here is that posed by the enormous number of elementary arithmetical operations involved in the construction of the energy matrices. Some idea of the difficulties can be inferred from the approximate shell-model studies of the isotopes of Sn by Kuo and the Barangers, ⁽⁴⁴⁾ where the unmodified Tabakin interaction operates within the identical-nucleon configurations $(2d_{5/2}, 1g_{7/2}, 3s_{1/2}, 2d_{3/2}, 1h_{11/2})^n$, $n = 12$ to 25. Since this model space already far outstrips the capacity for exact calculation, ⁽⁹⁷⁾ the Bogoliubov-Valatin quasi-particle approximation ⁽⁹⁸⁾ is used. It is found that the calculated energy levels of the even-mass Sn isotopes are much too closely spaced and that even-odd mass differences have roughly half their experimental values. Thus within the model space d spanned by particles within the five allowed orbits the Tabakin interaction is much too weak; it is shown in ref. 44 that similar results are obtained using as effective interaction a Hamada-Johnston reaction matrix. This striking discrepancy is not due to the use of the quasi-particle approximation and must be handled by extension of the model space. It is found, however, that the necessary extension is frighteningly large. In order to produce reasonable qualitative agreement with experiment, twelve active orbits must be included in the shell-model calculation rather than five.

The conclusion is that only for light nuclei ($A < 40$) will sufficiently large complete shell-model calculations ever be possible to allow a detailed application of the reaction-matrix formalism of §§ 4–9. This comes about because the practical applicability of the reaction-matrix formalism demands that configurations bordering on the model space be susceptible to perturbative treatment; an impossibly severe strain is thereby imposed on available shell-model computing technique.

There is of course no good reason to insist that extensions of the model space must be made by allowing a few more active orbits into the calculation and then constructing complete energy matrices. Indeed, the process is inherently wasteful. It is clear, in fact, that most of the physics of a given problem will be found in the model space first chosen. The first extension of the model space, in which one or two more orbits are allowed an active role, achieves 10% corrections at the expense of an increase in dimensions by at least an order of magnitude. The next extension improves matters by 5% while dimensions increase by more than two orders of magnitude. A law of diminishing returns is in operation.

Techniques involving the use of intrinsic states provide a more economical way of extending shell-model vector spaces. To illustrate the method, consider the extended shell-model calculations suggested above for F^{18} . It is unnecessary to construct all the states of the $(4p, 2h)$ configurations $1p^{-2}(1d, 2s)^4$; the relevant deformed states of these configurations can be constructed by projection of angular-momentum eigenstates from the intrinsic state $|\chi\rangle$ made by removing a $T = 0$ nucleon pair from the highest $1p$ deformed single-particle state in the intrinsic ground state of Ne^{20} . The resulting extension of the F^{18} model space is symbolized by

$$(1d, 2s)^2_J \rightarrow (1d, 2s)^2_J + P_J |\chi\rangle \quad (85)$$

where $J = 1, 3$ or 5 . The extension to more than one intrinsic state is obvious.

Such intrinsic-state methods (⁹⁹) are useful here only if the necessary interaction-matrix elements can be computed directly from the properties of the intrinsic states; if it is necessary to expand the intrinsic states in the shell-model basis, calculate the energy matrix there and transform back again, nothing has been gained. The direct calculation of matrix elements is possible (¹⁰⁰) provided that the entire problem, including the part in the original model space, is treated within the intrinsic representation. There is not yet enough numerical experience with these techniques to indicate clearly how far they will extend the power of exact shell-model calculations; it is likely that they will continue to be most useful for light nuclei, where large deformations can be produced with relatively little configuration mixing.

Similar intrinsic-state techniques, based on projection of number-eigenstates from few-quasi-particle (⁹⁸) intrinsic states, have been shown (¹⁰¹) to provide a good approximation to identical-nucleon shell-model calculations. These calculations, however, evaluate the energy matrix by expansion in the shell-model basis and are therefore valueless in the present context. (¹⁰²)

One possible source of shell-model approximations does not seem to have been considered; it is the reaction-matrix formalism itself. Suppose that for a given many-particle system d_1 is the smallest model space large enough to permit a perturbative treatment of higher configurations; let $\mathfrak{g}_1$ be the effective interaction within d_1 . Suppose further that d_2 , a subspace of d_1 ($d_2 \subset d_1$), is the largest model space for which exact shell-model calculations are possible. Then consider the basic equations (23) and (24) of the embedding formalism of §4 with V replaced by $\mathfrak{g}_1$, $\mathfrak{g}$ replaced by $\mathfrak{g}_2$ (the effective interaction in d_2), the complete Hilbert space D of the system replaced by d_1 and with the model space d replaced by d_2 . These equations now specify the eigenvalue problem within the tractable space d_2 that reproduces the lowest eigenvalues of the intractable eigenvalue problem in d_1 . A useful framework is provided

for an average treatment of the higher configurations d_1-d_2 . The intermediate states $|\phi_k\rangle$ in the appropriate form of eq. (24) are not to be treated individually; rather each configuration is to be replaced by a distribution of known width and centroid position. The single-particle energies ϵ_k in the energy denominators of eq. (24) can be replaced by the centroid energies $\langle H \rangle_k$ by a suitable geometric resummation. The widths and centroid energies are calculated from the known interaction s_1 by the methods of ref. 103. The reaction-matrix formalism itself therefore provides a way to treat the configurations between d_1 and d_2 in a better approximation than lowest-order perturbation theory but in less detail than that involved in a straightforward extension of the model space.

It is probable, then, that available computing techniques and methods of approximation do not make possible large enough shell-model calculations to apply the reaction-matrix formalism to many-particle systems in heavy nuclei. Thus the phenomenological shell model and the reaction-matrix formalism will continue to meet in light nuclei ($A \leq 40$) and in few-particle systems. Out of these meetings may emerge an extrapolated version of the many-particle shell model, with parameters firmly grounded in nuclear many-body theory.

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Table 1. Measured and calculated(⁸⁰) level energies in F¹⁹. The table gives the excitation energy for the excited states and the energy defined by eq. (81) for the ground state. All energies are in MeV.

Spin	Measured Energy	Calculated Energy
$\frac{1}{2}$	(-11.30)	(-11.49)
$\frac{5}{2}$	0.20	0.46
$\frac{3}{2}$	1.56	2.17
$\frac{9}{2}$	2.79	2.76
$\frac{1}{2}$		3.92
$\frac{5}{2}$		4.58
$\frac{7}{2}$		4.13

Table 2. Measured and calculated(⁸⁰) level energies in Ne²⁰. The table gives the excitation energy for the excited states and the energy defined by eq. (81) for the ground state. All energies are in MeV.

Spin	Measured Energy	Calculated Energy
0	(-24.00)	(-22.98)
2	1.63	1.61
4	4.25	4.41
0	6.75	6.74
2	7.46	7.43
0	8.60	8.63
6	8.79	8.49
4	9.11	9.22
8	11.99	12.03

Table 3. Changes in the calculated(⁸⁰) spectrum of O¹⁹ when a fit is forced to the energy of the 1⁺ state at 1.7 MeV in F¹⁸. The table gives the excitation energy for the excited states and the energy defined by eq. (81) for the ground state. All energies are in MeV.

Spin	Calculated Energies		Measured Energy
	with F ¹⁸ (1 ⁺)	without F ¹⁸ (1 ⁺)	
$\frac{5}{2}$	(-3.59)	(-3.64)	(-3.72)
$\frac{3}{2}$	0.35	0.07	0.10
$\frac{1}{2}$	1.25	1.48	1.47
$\frac{9}{2}$	2.39	2.65	2.78
$\frac{5}{2}$	2.99	3.17	3.15
$\frac{7}{2}$	1.51	2.87	

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⁴J. P. Elliott and A. M. Lane, ref. 2, pp. 245-287.

⁵See, for example, F. Villars, in Proceedings of the Enrico Fermi Summer School of Physics, Course XXIII, 1961 (Academic Press, Inc., New York, 1963). M. Jean, in Proceedings of the Enrico Fermi Summer School of Physics, Course XL, 1967 (Academic Press, Inc., to be published) (the present volume).

The idea is to define the single-particle potential U in eq. (2) in such a way as to cancel as much as possible of the two-body interaction $\bar{V}$. In diagrammatic language, U diagrams are made to cancel hierarchies of $\bar{V}$ diagrams. In Brueckner theory this compensation principle still leaves a wide choice of definitions for U . (See ref. 26.) Once U has been defined, its presence in diagrammatic calculations is felt in the energy denominators and in the form of rules that certain classes of $\bar{V}$ diagrams should not be drawn. Such rules are not discussed in these lectures. They will, however, always be assumed to exist somewhere in the background and the residual interaction V will be loosely described as 'the free-nucleon interaction' instead of 'the residual part of the free-nucleon interaction.'

⁶B. H. Brandow, Revs. Mod. Phys. 39 (October 1967), in press. §§ 4 and 5 of these lectures follow Brandow's treatment of effective interactions in general outline and, to some extent, in notation. Note, however, that Brandow uses the symbol D for the model space; these lectures use D for the complete Hilbert space of the system, d for the model space.

⁷R. J. Eden and N. C. Francis, Phys. Rev. 97, 1366 (1955).

⁸C. Bloch and J. Horowitz, Nucl. Phys. 8, 91 (1958). Bloch and Horowitz derive eqs. (23) and (24) as a form of Brillouin-Wigner perturbation theory for degenerate systems.

⁹This is a characteristic feature of Brillouin-Wigner perturbation theory (See ref. 8).

¹⁰For application to real physical situations, this argument should be recast, by partial summation, in terms of the reaction matrix. This recasting, however, does not alter or vitiate the point being made.

¹¹The treatment here follows ref. 6. See also ref. 8 and B. D. Day, Ph. D. thesis (Cornell University, 1964), unpublished.

¹²J. Goldstone, Proc. Roy. Soc. A239, 267 (1957). In the present lectures a V -interaction is represented by a dotted line. Baranger's lectures (ref. 35), which treat such diagrams in great detail, use wavy lines for V -interactions.

¹³Such techniques are discussed and applied extensively in ref. 6.

¹⁴Note that Goldstone (ref. 12) and Bloch-Horowitz (ref. 8) use the adjective 'connected' for linked graphs with no external lines. There is no need to maintain this distinction here.

¹⁵Linked-cluster expansions have been proved in various ways and by many authors. Some of the earlier references are:

J. Goldstone (ref. 12)

N. M. Hugenholtz, *Physica* 23, 481 (1957)

J. Hubbard, *Proc. Roy. Soc. A* 240, 539 (1957)

F. Coester, *Nucl. Phys.* 7, 421 (1958)

C. Bloch, *Nucl. Phys.* 7, 451 (1958)

C. Bloch, and J. Horowitz (ref. 8)

¹⁶Untouched valence lines should not be counted as unlinked parts of a diagram; their explicit presence is merely conventional, a result of a particular choice of reference state.

¹⁷T. Morita, *Prog. Theor. Phys.* 29, 351 (1963).

¹⁸Webster's New World Dictionary states that realistic means "practical rather than visionary"!!

¹⁹K. A. Brueckner, C. A. Levinson, and H. M. Mahmoud, *Phys. Rev.* 95, 217 (1954); K. A. Brueckner, *Phys. Rev.* 96, 508 (1954); K. A. Brueckner, *Phys. Rev.* 97, 1353 (1955).

²⁰See, for example, H. A. Bethe (ref. 3); R. J. Eden in Nuclear Reactions, Volume 1, P. M. Endt and M. Demeur, ed., (North-Holland Publishing Company, Amsterdam, 1959).

²¹Note that this choice of basis differs from that discussed in §3, in that total angular momentum is not specified. The inclusion of angular momentum in the subsequent arguments is so straightforward that this change of labelling for the basis states is of no consequence.

²²Most techniques used in 'finite-nucleus' calculations are adaptations from nuclear-matter calculations. See ref. 35.

²³Provided they are heavy enough. The 1p contributions in O^{18} and F^{18} ought to be calculated.

²⁴See, however, section III of ref. 3.

²⁵For example, 3p-1h and 4p-2h states. See §7.

²⁶ See section 2 of H. A. Bethe, B. H. Brandow and A. G. Petschek, Phys. Rev. 129, 225 (1963).

²⁷ J. F. Dawson, I. Talmi and J. D. Walecka, Ann. Phys. 18, 339 (1962); A. Kallio and K. Kolltveit, Nucl. Phys. 53, 87 (1964); S. Kahana and E. Tomusiak, Nucl. Phys. 71, 402 (1965); C. Shakin and M. Hull, Phys. Lett. 19, 506 (1965); see also refs. 32, 33, 41, and 44.

²⁸ The fact that the single-particle energy splittings for neutrons (O^{17}) and for protons (F^{17}) are slightly different is ignored. Its inclusion would mix isobaric spins, but only slightly.

²⁹ This is compensated by the inclusion in eq. (65) of the term $-2(B.E.(O^{17}) - B.E.(O^{16}))$ and the corresponding term $-2(B.E.(F^{17}) - B.E.(O^{16}))$ in eq. (66).

³⁰ T. Hamada and I. D. Johnston, Nucl. Phys. 34, 382 (1962).

³¹ F. Tabakin, Ann. Phys. 30, 51 (1964).

³² T. T. S. Kuo, Nucl. Phys. (to be published).

³³ T. T. S. Kuo, and G. E. Brown, Nucl. Phys. 85, 40 (1966).

³⁴ Kuo's paper (ref. 32) is entitled "State-dependence of Shell-Model Reaction-Matrix Elements". Kuo's state-dependence is not the E_v -dependence discussed here and in § 4; the states to which Kuo is referring are the basis states $|v_1 v_2\rangle$ of the model space and not the eigenstates of the shell-model problem.

³⁵ M. Baranger, in Proceedings of the Enrico Fermi Summer School of Physics, Course XL, 1967 (Academic Press, to be published) (the present volume).

³⁶C. W. Wong, Nucl. Phys. (to be published).

³⁷The physical basis of the plane-wave approximation is that the main contributions to the reaction matrix come from 2-particle states of high relative momentum; in such states the kinetic energy is much larger than the potential energy.

³⁸second order, that is, in the uncorrected reaction matrix.

³⁹This is not how Kuo (ref. 32) presents his results. He first gives spectra calculated with the uncorrected (plane wave) reaction matrix as effective interaction. He then includes (3p, 1h) corrections and, finally, adds on the special 2p correction under consideration together with (4p, 2h) corrections.

⁴⁰This is shown for attractive Yukawa interactions in section X of ref. 3. Of course, the Tabakin interaction is very different from an attractive Yukawa interaction. It would be interesting, in fact, to examine the solution of a reaction-matrix equation for the Tabakin potential.

⁴¹D. M. Clement and E. U. Baranger, Nucl. Phys. (to be published).

⁴²The experimental references are given in ref. 80.

⁴³L. A. König, J. H. E. Mattauch and A. H. Wapstra, Nucl. Phys. 31, 18 (1962).

⁴⁴T. T. S. Kuo, E. U. Baranger and M. Baranger, Nucl. Phys. 81, 241 (1966).

⁴⁵There are, however, many points in their calculation at which Clement and Baranger (ref. 41) make approximations similar to those that appear in Kuo's calculation (ref. 32).

⁴⁶R. P. Lynch and T. T. S. Kuo, Nucl. Phys. A95, 561 (1967).

⁴⁷Lynch and Kuo (ref. 46) use the methods of ref. 33 rather than the improved techniques of ref. 32. The additional errors that enter are probably unimportant because they should be of similar size in the three different reaction matrices that arise from the three different free-nucleon interactions.

⁴⁸Compare, for example, refs. 32 and 33. The interaction potential is found in ref. 33 to contribute -340 MeV. to the binding energy of O^{16} . Ref. 32 using the same free-nucleon interaction and a slightly improved method of calculating the reaction matrix, gives -306 MeV for this potential energy.

⁴⁹and to other effects ignored here—such as the proper choice of single-particle energies and wave functions.

⁵⁰Compare, for example, the Ni^{58} results of R. D. Lawson, M. H. Macfarlane and T. T. S. Kuo, Phys. Lett. 22, 168 (1966)

⁵¹G. F. Bertsch, Nucl. Phys. 74, 234 (1965).

⁵²The notation for core, valence and empty orbits is given in Fig. 6.

⁵³See section 4.2 of ref. 33.

⁵⁴Note the two unconnected uses of the symbol ω —here and in the phrase "excitation energy $2\hbar\omega$."

⁵⁵Bertsch (ref. 51) shows that, with the 3p-1h correction to the single-particle energy properly eliminated, the remaining 3p-1h effects add a net repulsion in states with $T = 1$ and high J , a net attraction in states with $T = 1$ and low J and have little influence in states with $T = 0$.

⁵⁶These small effects on the 2-particle spectra can of course have large effects in many-particle spectra. In particular, the fact noted by Bertsch

(ref. 51) that (3p, 1h) corrections are repulsive in states of high J and $T = 1$ results in a large repulsive correction to combinations of $T = 1$ matrix elements of the form $\sum_J (2J + 1) \langle v_1 v_2 J | \mathcal{V} | v_1 v_2 J \rangle$. This has an effect on the ground-state binding energies of identical-nucleon systems which is both large and in agreement with experiment. (See pp. 637 and 638 of M. H. Macfarlane (ref. 2)).

⁵⁷P. Federman and I. Talmi, Phys. Lett. 15, 165 (1965); Phys. Lett. 19, 490 (1965).

⁵⁸I.e., $|\beta/a|^2$ in eq. (56) is about .3.

⁵⁹This point is examined further in §8 and §11.

⁶⁰Clement and Baranger (ref. 41) in fact do not compute (4p, 2h) corrections. However, it is reasonable to suppose that such corrections would be similar to those found by Kuo (ref. 32) in view of the similarity of the bare reaction matrices and of the (3p, 1h) corrections.

⁶¹A clear discussion of such intrinsic states and of their projected J-components is given in ref. 62.

⁶²H. G. Benson and J. M. Irvine, Proc. Phys. Soc. (London) 89, 249 (1966).

⁶³L. Zamick, Phys. Lett. 19, 580 (1965); G. E. Brown and A. M. Green, Nucl. Phys. 85, 87 (1966).

⁶⁴T. Inoue, T. Sebe, K. K. Huang and A. Arima, Nucl. Phys. A99, 305 (1967).

⁶⁵The number quoted in ref. 64 is in fact 1.34 MeV. It is, of course, reliable only to within 1 or 2 MeV.

⁶⁶Except the 3^+ state at 5.37 MeV. However, the deformed intrinsic states of interest here have no $J = 3^+$, $T = 1$ components.

⁶⁷A. Kallio and A. M. Green, Nucl. Phys. 84, 161 (1966).

⁶⁸ Hole-particle matrix elements are related to particle-particle matrix elements by the recoupling transformation given in eq. (II. 46) of M. H. Macfarlane, ref. 2.

⁶⁹ N. de Takacsy, Nucl. Phys. A95, 505 (1967).

⁷⁰ H. A. Bethe, Phys. Rev. 138B, 804 (1965).

⁷¹ B. D. Day, Phys. Rev. 151, 826 (1966).

⁷² See the discussion in Chapter XII, section 1 of ref. 1. Compare fig. 61 of ref. 1 with fig. 16 of these lectures.

⁷³ Except in the crude approximation $\mathfrak{g} \approx G$, where G is either an uncorrected reaction matrix (ref. 44) or a 2-body reaction matrix with (3p, 1h) corrections (ref. 50). These calculations emphasize that huge additional configuration-mixing effects exist and that many-particle spectra are more sensitive to errors in G than are the 2-particle spectra.

⁷⁴ Irrelevant magnetic quantum numbers are omitted.

⁷⁵ This method was first used by Bacher and Goudsmit in atomic spectroscopy: R. F. Bacher and S. Goudsmit, Phys. Rev. 46, 948 (1934).

It was then applied to calculations of relative nuclear binding energies about twenty years later:

S. Goldstein and I. Talmi, Phys. Rev. 102, 589 (1956).

I. Talmi and R. Thieberger, Phys. Rev. 103, 718 (1956).

Applications to nuclear spectra are discussed by Talmi and Unna:

I. Talmi and I. Unna, Ann. Rev. Nucl. Science, Vol. 10, 353 (1960).

⁷⁶ The two-body matrix elements can be determined directly from the two-particle spectra only for the single-shell configurations j^2 .

⁷⁷ Many local minima exist in the 16-dimensional parameter space. The fit must be guided to a sensible solution by starting the minimization procedure in a physically reasonable region of parameter space.

⁷⁸Construction of the fitting function of eq. (80) requires the establishment of a one-to-one correspondence between calculated and observed states. This is done separately for each nucleus and for each spin, working upwards in energy. Thus the lowest calculated state of spin J is identified with the lowest observed state of spin J ; the next lowest calculated state of spin J is identified with the next lowest observed state of spin J , and so on. For a given nucleus, the process stops when a state of unknown spin is encountered.

⁷⁹Experimental references are given in ref. 80.

⁸⁰A. Arima, S. Cohen, R. D. Lawson and M. H. Macfarlane, submitted to Nucl. Phys.

⁸¹The indications from the phenomenological fit and from the discussion in §§7 and 8 are that the 2^+ state at 2.5 MeV in F^{18} does not have a particularly large deformed component.

⁸²In practice, of course, moments, transition rates and reaction cross-sections will be available to assist the study of configuration structure.

⁸³J. P. Elliott and B. H. Flowers, Proc. Roy. Soc. A229, 536 (1955). This calculation yields an eigenvector for the lowest $\frac{3}{2}^+$ state in F^{19} that has more than 50% of its intensity in the configurations $(d_{\frac{5}{2}}^2) d_{\frac{3}{2}}$ and $d_{\frac{5}{2}} d_{\frac{3}{2}} s_{\frac{1}{2}}$.

⁸⁴It is assumed here that the argument is not spoiled by the fact that the calculations of §§7 and 8 include the $d_{\frac{3}{2}}$ orbit while the phenomenological calculation does not. This probably influences the states of Ne^{20} to a considerable extent and also some of the levels in F^{19} . However, the main brunt of the discussion falls on the spectra of O^{18} and F^{18} where $d_{\frac{3}{2}}$ admixtures are small.

⁸⁵S. Cohen, R. D. Lawson and J. M. Soper, Phys. Lett. 21, 306 (1966).

⁸⁶In practice there are considerable uncertainties about the precise form of T . See A. de Shalit in Proceedings of the Enrico Fermi Summer School of Physics, Course XXIII, 1961 (Academic Press, Inc., New York, 1963).

⁸⁷A. Arima and H. Horie, Prog. Theor. Phys. 11, 509 (1954); H. Noya, A. Arima and H. Horie, Prog. Theor. Phys. (Supplement) 8, 33 (1958).

⁸⁸H. A. Mavromatis, L. Zamick and G. E. Brown, Nucl. Phys. 80, 545 (1966).

⁸⁹I.e., one that has the correct qualitative properties but does not attempt precise fits to the nucleon-nucleon scattering data.

⁹⁰In the reaction-matrix formalism T_{eff} may contain 2-, 3-, ... body operators.

⁹¹See, for example, de Shalit and Talmi, ref. 2.

⁹²Cohen and Kurath obtain impressive agreement with experiment for magnetic moments and β -decay ft-values of 1p-shell nuclei ($6 \leq A \leq 14$): S. Cohen and D. Kurath, Nucl. Phys. 73, 1 (1965).

This seems to be the zenith of achievement in the shell-model treatment of transition rates, both in quality of agreement with experiment and in the quantity of data fitted. For heavier nuclei, the shell model with unmodified transition operators is much less successful.

⁹³E.g., the self-consistent calculation of single-particle properties.

⁹⁴Or slightly modified by a second-order perturbative correction.

⁹⁵Villars, da Providencia and Shakin have shown that a unitary transformation can be found that transforms a given hard-core two-body interaction into a smooth interaction (without hard cores) with a predominant two-body part and many-body corrections. They argue that the many-body terms are negligible and show that the two-body part of the transformed Hamiltonian is the Hermitian part of the reaction matrix of the hard-core interaction:

F. Villars, ref. 5;

J. da Providencia and C.M. Shakin, Ann. Phys. (N. Y.) 22, 133 (1963);

Nucl. Phys. 65, 54 (1965); Nucl. Phys. 65, 75 (1965).

⁹⁶ The manner in which small differences in two-body matrix elements can lead to large difference in many-particle spectra can be seen in the Ni calculations of ref. 50.

⁹⁷ There are, for example, more than 10,000 states with spin 2 for $n = 16$ (the middle of the shells).

⁹⁸ M. Baranger, Phys. Rev. 120, 957 (1960).

⁹⁹ D. Kurath and L. Picman, Nucl. Phys. 10, 313 (1959); C. A. Levinson and I. Kelson, Phys. Rev. 134, B269 (1964).

¹⁰⁰ G. Ripka, in Lectures in Theoretical Physics, Volume VIII-C, (University of Colorado Press, 1966); I. Kelson, Nucl. Phys. 89, 387 (1966).

¹⁰¹ A. K. Kerman, R. D. Lawson, and M. H. Macfarlane, Phys. Rev. 124, 162 (1961); M. H. Macfarlane, ref. 2.

¹⁰² Attention is confined here to shell-model calculations in which good quantum numbers such as angular momentum and particle-number are conserved. This in no way denies the usefulness of unprojected quasi-particle techniques in phenomenological shell-model calculations and in the calculation of average properties of nuclei with realistic interactions.

¹⁰³ J. B. French and H. Banerjee, Phys. Lett 23, 245 (1966); J. B. French, Phys. Lett. 23, 248 (1966); F. S. Chang, J. B. French and K. F. Ratcliff, Phys. Lett. 23, 251 (1966).

FIGURE CAPTIONS

- Fig. 1 Rough sketch of the single-particle spectrum underlying the nuclear shell model.
- Fig. 2 Schematic illustration of the shell model's basic act of truncation.
- Fig. 3 A physical situation in which a strongly state-dependent effective interaction might be expected.
- Fig. 4 Diagrams that contribute to the effective interaction in the special case $n = 3$. V-interactions are represented by dotted lines.
- Fig. 5 An unlinked valence diagram for $n = 4$.
- Fig. 6 Core, valence and empty single-particle states.
- Fig. 7 A contribution to the effective interaction for $n = 2$ in which one valence nucleon is excited into an empty orbit.
- Fig. 8 The equation for the reaction matrix.
- Fig. 9 Calculated and observed states of positive parity in O^{18} . The spectrum labelled G_T is that calculated by Clement and Baranger⁽⁴¹⁾ using as interaction a reaction matrix derived from the free-nucleon potential of Tabakin.⁽³¹⁾ The spectrum labelled $\bar{G}$ is calculated from a reaction matrix derived by Kuo⁽³²⁾ from the free-nucleon potential of Hamada and Johnston.⁽³⁰⁾
- Fig. 10 Calculated and observed states of positive parity in F^{18} . The significance of the labels G_T and $\bar{G}$ on the calculated spectra is given in the caption to Fig. 9.
- Fig. 11 Core-excited diagrams that contribute to the effective interaction in two-particle shell-model systems.
- Fig. 12 A core-excited contribution to a single-particle energy.
- Fig. 13 Calculated and observed spectra of O^{18} . The label $[3p, 1h]$ indicates that in the pertinent shell-model calculation the effective interaction is a reaction matrix with perturbative corrections for $(3p, 1h)$ intermediate states; the label $[4p, 2h]$ has a similar interpretation. The significance of the labels G_T and $\bar{G}$ is given in the caption to Fig. 9.

- Fig. 14 Calculated and observed spectra of F^{18} . The significance of the labels on the calculated spectra is given in the caption to Fig. 13.
- Fig. 15 Diagrams that contribute to the effective interaction in 3-particle shell-model systems.
- Fig. 16 3-body contributions to the effective interaction in 3-particle systems.
- Fig. 17 Calculated and observed spectra of O^{18} . The "model" spectrum is the phenomenological best fit of Arima, et al. ⁽⁸⁰⁾
- Fig. 18 Calculated and observed spectra of F^{18} . The "model" spectrum is the phenomenological best fit of Arima, et al. ⁽⁸⁰⁾

_____	1h 11/2
_____	2d 3/2
_____	3s 1/2
_____	1g 7/2
_____	2d 5/2

_____	1g 9/2
_____	2p 1/2
_____	1f 5/2
_____	2p 3/2
_____	1f 7/2

_____	1d 3/2
_____	2s 1/2
_____	1d 5/2
_____	1p 1/2
_____	1p 3/2
_____	1s 1/2

UNPERTURBED
STATES $|\Phi_k\rangle$
OF CONFIGURATIONS e

STATES $|\Psi^r\rangle$
TO BE TREATED
WITHIN d

COLLECTIVE STATE $|\Psi_e^0\rangle$

$\langle H_0 \rangle_k$

$\langle H_0 + V \rangle_e^0$

a)

b)

c)

d)

Fig. 5

UNOCCUPIED STATES
 $a, b, \dots$

VALENCE STATES
 $v_1, v_2, \dots$

OCCUPIED STATES
 $A, B, \dots$

Fig. 9

a)

b)

Fig. 12

Fig. 14

a)

b)

Fig. 15

Fig. 17

Fig. 18