THEORY OF OVERLAP FUNCTIONS

I SINGLE PARTICLE SUM RULES AND CENTRE-OF-MASS CORRECTIONS

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Abstract

Model-independent relations are obtained between the overlap functions defined by projecting onto one another states of nuclei differing by one particle. Exact partial sum rules for spectroscopic factors obtained from one-nucleon transfer reactions on non-zero spin target nuclei are derived, and some applications to experiments on $2s_{1/2}$ and $1f_{7/2}$ neutron transfer are considered.

A straightforward derivation is given of the $1/A$ corrections to the sum rules including the correction to the total single particle sum rule of MacFarlane and French. It is shown that the corrections are not negligible for light nuclei, and the ways in which they affect the interpretation of knockout reactions in the $1p$ shell and transfer reactions on ^{16}O and ^{40}Ca are discussed.

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1. Introduction.

There are basically two main approaches to the theoretical study of many-fermion systems. The first approach, which derives from atomic physics, is to construct model many-body wave functions for a system with a given number of particles. All physically observable quantities such as energies and expectation values of electromagnetic operators are then determined and can be compared to experiment. This is the traditional approach of the nuclear shell model and its extensions.

The second main approach, which is used extensively in the physics of infinite many-body systems such as solids, is to examine the system and its properties in the order of increasing numbers of particles. Thus, one starts with one-body motion and then introduces two-body correlations, three-body correlations and so on. Mathematically, the system is described in terms of density matrices of increasing order. This approach is naturally oriented towards the description of the interaction of one particle or a pair of particles in the system with an external field or an external particle which can be observed experimentally.

Of course, if one knows total wave functions, as in the first approach, all the density matrices and thus external interactions are in principle calculable. However, there are two criticisms which can be made of these calculations. Firstly, one has more information about the system than can easily be compared with experiment. For example in nuclear physics, apart from angular momentum correlations between particles which are very important, it is very difficult to find experiments which detect even two-body correlations. These are the correlations which arise from 'holes' in the nuclear wave function. Secondly, the sensitivity

of observed one and two nucleon properties to changes in the total wave functions is not immediately apparent. One attempt to discuss this sensitivity in the nuclear shell model has been made by Lawson and Soper.¹⁾

This paper is the first of a series in which we attempt to construct a version of the second approach for use in nuclear physics. The first thing that strikes one about the theoretical interpretation of a large fraction of nuclear physics experiments is that the crucial quantity involving bound states that enters into the theory is an overlap function obtained by projecting the wave functions of neighbouring nuclei onto one another. One-nucleon overlap functions occur in one-nucleon transfer theories of stripping and pickup reactions and also in the theory of nucleon elastic and inelastic scattering. Two-nucleon overlap functions appear in the theory of two-nucleon transfer reactions and also in theories of the interaction of external particles such as mesons with nuclei which would in principle determine two-body correlations.

The importance of one-nucleon overlap functions especially in (p-2p) knockout reactions was realized by Berggren²⁾ who derived some of their properties. We have already extended his work to discuss sum rules^{3,4)}, derive a fundamental theorem⁵⁾ and produce modified Hartree-Fock equations⁶⁾. The theorem of ref. ⁵⁾ is basic to our work and indeed to any description of a finite fermion system in terms of single particle orbits. One way of stating it is, if spectroscopic factors, which are the normalizations of the overlap functions, are less than unity, the overlap functions are not linearly independent and can be expressed as a linear combination of a smaller number of single particle wave functions. The single particle wave functions are to be approximately identified with those of the

shell model. The appropriate experiments on the direct addition or removal of an electron are lacking in atomic and molecular physics but would directly test the existence of single particle orbitals there.

We speculate that there exist general theorems for finite fermion systems such as, if there are constants of the motion or operators such as total angular momentum which commute with the Hamiltonian, then there exist overlap functions with spectroscopic factors less than unity. These would arise from the mixing of degeneracies caused by angular momentum coupling. It would be nice, but possibly not very useful, to prove such theorems.

The continuing work most closely related to ours is that of French and his collaborators⁷⁻¹³ (other references will be found in the ones quoted) who have a somewhat similar philosophy to the second approach. French works mainly within the context of the shell model and examines the properties of distributions of operator products. He obtains single particle sum rules and properties of the energy weighted distribution of spectroscopic factors, for example. His technique is basically that of second quantization.

Our approach differs from that of French in several respects. Firstly we work directly with overlap functions defined in the co-ordinate representation and obtain exact relations as opposed to approximate ones. Our technique uses explicit antisymmetrization as opposed to second quantization. This has several advantages in that there is no need to adopt a shell-model representation at the start; the latter arises naturally as the lowest order approximation. Also, continuum states can be included and it is straightforward to obtain $1/A$ corrections, as in this paper. All quantities appearing in the theory, namely

overlap functions and spectroscopic factors, are used in the analysis of experiments. We also have obtained new results^{5,6)} including sum rules for two-nucleon transfer reactions¹⁴⁾.

The partial sum rules obtained in this paper are the exact versions of ones obtained by French⁸⁾. They have not received the applications in nuclear physics so far that they deserve and do not appear to be widely known among experimentalists. Using both French's work and our own far more use can be made of the vast mass of data on one-nucleon transfer reactions that has accumulated in nuclear physics.

It is appropriate to discuss some of the material which we hope to present in these papers. In this first paper we essentially generalize previous work^{3,4,5)} to obtain orthogonality relations between overlap functions, partial sum rules for spectroscopic factors obtained from reactions on non-zero spin nuclei and $1/A$ corrections to the sum rules, including those for the familiar total sum rule of MacFarlane and French¹⁵⁾. Some applications to experimental results are discussed.

In the second paper we will show that all one-body properties of nuclei, such as the density, electromagnetic moments and transition rates can be explicitly given in terms of overlap functions, thus extending the idea of Berggren²⁾. We also intend to discuss in detail continuum contributions to single particle sum rules, a subject on which some progress has already been made^{16,17)}. Considerable extension of previous work on obtaining dynamical equations⁶⁾ is also possible. The introduction of correlations via effective interactions needs to be made. We also think it possible to derive 'particle-hole' theories from our exact equations by making truncations and approximations. There is also a lot of work to be done on two-nucleon overlap functions. Altogether we

anticipate gaining considerably more insight into nuclear physics through a microscopic approach based on overlap functions.

In this first paper we begin, in sect. 2 by defining overlap functions and the notation that we are going to use. In sect. 3 we obtain a large number of exact relations between overlap functions, ignoring for the time being $1/A$ corrections. Some approximate orthogonality relations are obtained for use when a given $(j\ell)$ shell is 'closed'. The sense in which a shell is 'closed' follows from previous work⁵⁾ and is briefly discussed.

Partial sum rules, which approximately reduce to those of French⁸⁾, are obtained in sect. 4 where we also point out their applications to $\ell = 0$ transfer reactions and to reactions on $1f_{7/2}$ shell nuclei. In sects. 5 and 6 we consider $1/A$ corrections to the sum rules. The algebra is mostly performed in sect. 5 which can safely be ignored by those seeking the results. These are obtained, using a simple model, in sect. 6. We show that the $1/A$ corrections are not negligible for light nuclei and discuss corrections for knockout $(p-2p)$ reactions in the $1p$ shell and sum rule corrections for reactions on ^{16}O and ^{40}Ca . Finally in sect. 7 we discuss the results obtained and offer our conclusions.

2. Definitions and Notation.

In this section we define the overlap functions and establish some of the notation to be used throughout these papers. In general the notation follows established practice in the literature but we shall, wherever possible, shorten undue labelling to make subsequent equations more concise.

We use isospin notation so that all nuclear wave functions are anti-symmetric under the interchange of all co-ordinates $i(\underline{r}_i, \underline{p}_i, \underline{z}_i)$ and $j(\underline{r}_j, \underline{p}_j, \underline{z}_j)$ of any pair of particles. Neutrons are taken to have $t_3 = +1/2$ and in general we shall assume that for the bound state wave functions, isospin is a good quantum number so that the wave functions are labelled accordingly. It would be easily possible, but lead to very cumbersome equations, to relax this restriction and regard the states as mixtures of wave functions with different total isospin.

Bound state wave functions of $A-1$, A and $A+1$ particle nuclei are denoted by $\Psi_\alpha(1 \dots A-1; \underline{J}_\alpha M_\alpha T_\alpha T_{3\alpha})$, $\chi_\alpha(1 \dots A; \underline{J}_\alpha M_\alpha T_\alpha T_{3\alpha})$ and $\Psi_n(1 \dots A+1; \underline{J}_n M_n T_n T_{3n})$ respectively. For simplicity, the labelling α will be extended to cover all the continuum states of the $(A-1)$ particle system. Any summation over α is then understood to include integration over E_α and summation over any other variables needed to specify the states at E_α .

Continuum states of $(A+1)$ - particles are here denoted by $\Psi_n^{(+)}(1 \dots A+1; \underline{k}_n)$, where n labels the incident channel for the scattering state with incident momentum $\underline{k}_n$. More than one momentum may be needed to specify the state but, for simplicity, we only use here one label, $\underline{k}_n$. Also n includes specification of any spin quantum numbers needed to label the states. This labelling system will

be elaborated elsewhere when the continuum states are discussed in detail.

In terms of the above definitions the unit operators in the (A-1)- and (A+1)-particle spaces are, respectively,

$$I_{A-1} = \sum_{\alpha M_{\alpha}} |\Psi_{\alpha}(1 \dots A-1; J_{\alpha} M_{\alpha} T_{\alpha} T_{3\alpha}) \rangle \langle \Psi_{\alpha}(1 \dots A-1; J_{\alpha} M_{\alpha} T_{\alpha} T_{3\alpha})| \quad (1)$$

$$I_{A+1} = \sum_{n M_n} |\Psi_n(1 \dots A+1; J_n M_n T_n T_{3n}) \rangle \langle \Psi_n(1 \dots A+1; J_n M_n T_n T_{3n})| \\ + \sum_n \int d^3 k_n |\Psi_n^{(c)}(1 \dots A+1; k_n) \rangle \langle \Psi_n^{(c)}(1 \dots A+1; k_n)| \quad (2)$$

Overlap functions between the nuclei differing by one nucleon are defined by

$$A^{1/2} \langle \Psi_{\alpha}(1 \dots A-1; J_{\alpha} M_{\alpha} T_{\alpha} T_{3\alpha}), \chi_r(1 \dots A; J_r M_r T_r T_{3r}) \rangle \\ = \sum_{j l m t_3} (J_{\alpha} M_{\alpha} j m | J_r M_r) (T_{\alpha} T_{3\alpha} \frac{1}{2} t_3 | T_r T_{3r}) \quad (3)$$

$$\Theta_{\alpha r}(j l t_3) \phi_{\alpha r}(z_A - B_{A-1}; j l m t_3),$$

$$(A+1)^{1/2} \langle \chi_r(1 \dots A; J_r M_r T_r T_{3r}), \Psi_n(1 \dots A+1; J_n M_n T_n T_{3n}) \rangle$$

$$= \sum_{j l m t_3} (J_r M_r j m | J_n M_n) (T_r T_{3r} \frac{1}{2} t_3 | T_n T_{3n})$$

$$\Theta_{rn}(j l t_3) \phi_{rn}(z_{A+1} - B_A; j l m t_3), \quad (4)$$

$$\begin{aligned}
 (A+1)^{1/2} < \chi_r(1 \dots A; J_r M_r T_r T_{3r}), \Psi_n^{(q)}(1 \dots A+1; B_n) > \\
 = \Phi_{rn}^{(q)}(\tau_{A+1} - B_A; B_n), \quad (5)
 \end{aligned}$$

where the integrations are over all internal co-ordinates of the smaller nucleus so that the normalized functions $\phi_{\alpha r}$ and ϕ_{rn} are functions of the variables indicated. Specifically, for example,

$$\begin{aligned}
 \phi_{\alpha r}(\tau_A - B_{A-1}; j l m t_3) &= \phi_{\alpha r}(|\tau_A - B_{A-1}|; j l t_3) \\
 [Y_l(\tau_A - B_{A-1}) X^{1/2}(\tau_A)]_m^j &X_{t_3}^{1/2}(\tau_A).
 \end{aligned}$$

where the square brackets denote vector coupling in the order indicated and $\phi_{\alpha r}(|\tau_A - B_{A-1}|; j l t_3)$ is a normalized radial function;

$$\int_0^\infty dr \, r^2 \phi_{\alpha r}^2(r; j l t_3) = 1. \quad (6)$$

The phases of the states are chosen so that both $\Theta_{\alpha r}$ and Θ_{rn} are real, when the usual spectroscopic factors are

$$\begin{aligned}
 S_{\alpha r}(j l t_3) &= \Theta_{\alpha r}^2(j l t_3) \\
 S_{rn}(j l t_3) &= \Theta_{rn}^2(j l t_3) \quad (7)
 \end{aligned}$$

The continuum overlap function, $\Phi_{rn}^{(q)}(\tau_{A+1} - B_A; B_n)$, is not

normalized and its dependence on r implies a dependence on the quantum numbers, J_r, M_r, T_r, T_{3r} .

It is convenient and abbreviates our equations to absorb the isospin Clebsch-Gordon coefficients into the spectroscopic factors, so that we defined primed spectroscopic factors by

$$\begin{aligned}\theta'_{\alpha r} &= (T_{\alpha} T_{3\alpha} \frac{1}{2} t_3 | T_r T_{3r}) \theta_{\alpha r}, \quad S'_{\alpha r} = \theta_{\alpha r}'^2 \\ \theta'_{rn} &= (T_r T_{3r} \frac{1}{2} t_3 | T_n T_{3n}) \theta_{rn}, \quad S'_{rn} = \theta_{rn}'^2\end{aligned}\quad (8)$$

It is also useful to remove the angular, spin and isospin overlap functions and to this end we introduce a normalized function of these coordinates

$$\phi(\Omega_{\tilde{r}} \tilde{r} \tilde{r}; j l m t_3) = \left[Y_l(\tilde{r}) \chi^{\frac{1}{2}}(\tilde{r}) \right]_m^j \chi_{t_3}^{\frac{1}{2}}(\tilde{r}). \quad (9)$$

It is then easy to verify that the definitions (3) and (4) may be rewritten in the forms,

$$\begin{aligned}A^{\frac{1}{2}} < \left[\Psi_{\alpha} (1 \cdots A-1; J_{\alpha} T_{\alpha} T_{3\alpha}) \phi(\Omega_A, \tilde{r}_A, \tilde{r}_A; j l t_3) \right]_{M_r}^{J_r} \\ &\quad \chi_r (1 \cdots A; J_r M_r T_r T_{3r}) > \\ &= \theta'_{\alpha r} (j l t_3) \phi_{\alpha r} (1 \tilde{r}_A - B_{A-1}; j l t_3),\end{aligned}\quad (10)$$

$$\begin{aligned}
(A+1)^{1/2} &< \left[\chi_r(1 \dots A; J_r T_r T_{3r}) \phi(\Omega_{A+1}, \Sigma_{A+1}, \Xi_{A+1}; j l t_3) \right]_{M_n}^{J_n} \\
&\Psi_n(1 \dots A+1; J_n M_n T_n T_{3n}) > \\
&= \Theta'_{rn}(j l t_3) \phi_{rn}(|\Sigma_{A+1} - \Xi_A|; j l t_3), \quad (11)
\end{aligned}$$

where Ω_A, Ω_{A+1} refer to the co-ordinates $\Sigma_A - \Xi_{A-1}$ and $\Sigma_{A+1} - \Xi_A$, respectively.

One simple consequence of our definitions will be derived immediately. We have

$$A \langle \chi_s, \chi_r \rangle = A \delta_{rs} \delta_{J_r J_s} \delta_{T_r T_s} \delta_{M_r M_s} \delta_{T_{3r} T_{3s}}.$$

Inserting I_{A-1} given by eq. (1) and using the definitions (3) and (7), we obtain

$$\begin{aligned}
&\sum_{\alpha j l t_3} \Theta'_{\alpha s}(j l t_3) \Theta'_{\alpha r}(j l t_3) \int r^2 \phi_{\alpha s}(r; j l t_3) \phi_{\alpha r}(r; j l t_3) dr \\
&= A \delta_{rs} \delta_{J_r J_s} \delta_{T_r T_s} \delta_{M_r M_s} \delta_{T_{3r} T_{3s}} \quad (12)
\end{aligned}$$

The off-diagonal equations are orthogonality relations and the diagonal relation when $r=s$ is, from eq. (6),

$$\sum_{\alpha j l t_3} S'_{\alpha r}(j l t_3) = A \quad (13)$$

More generally, isospin operators can be included in the diagonal matrix element so that we have

$$\begin{aligned} \frac{N}{Z} &= \langle \chi_r, \sum_i \frac{1}{2} (1 \pm \tau_{3i}), \chi_r \rangle \\ &= \sum_{\alpha, j, l, t_3 = \pm 1/2} S'_{\alpha r}(j, l, t_3) \end{aligned} \quad (14)$$

Thus, sums of the spectroscopic factors as defined specify the numbers of nucleons in the nucleus. This is important, as will be seen in sect. 6, since the sum rules (for individual j, l, t_3) with centre-of-mass corrections do not have integer values.

3. Exact Relations between Overlap Functions.

In this section we generalise the technique previously used⁵⁾ to obtain the exact representation of any normalized single particle function in terms of the overlap functions defined in sect. 2. The generalization takes two forms. Firstly, we consider states of the A-particle nucleus with arbitrary spin and secondly we take off-diagonal elements between different states of the A-particle nucleus. In this section we shall then immediately take the first term in a $1/A$ expansion of the exact equations. The first order correction terms of order $1/A$ and their consequences for the sum rules are discussed in sects. 6 and 7.

An arbitrary normalised single particle function is defined by

$$\phi(A+1; j\ell m t_3) = \phi(|x_{A+1} - R_A|; j\ell t_3) \\ \left[Y_\ell(x_{A+1} - R_A) X^{\frac{1}{2}}(\Sigma_{A+1}) \right]_m^j X^{\frac{1}{2}}_{t_3}(\Sigma_{A+1}), \quad (15)$$

where the radial wave function is normalized with respect to integration over $|x_{A+1} - R_A|$.

A coupled antisymmetric function of $(A+1)$ -particle co-ordinates is then constructed from an arbitrary bound state χ_r of the A-particle nucleus.

$$\Phi_r(1 \dots A+1; [J_r, j\ell]_m^J T_r T_{3r} \frac{1}{2} t_3) = (1 - \sum_{i=1}^A P_{i,A+1}) \left[\chi_r(1 \dots A; J_r T_r T_{3r}) \phi(A+1; j\ell t_3) \right]_m^J \quad (16)$$

where P_{ij} is the permutation operator which interchanges all coordinates of the two particles i and j .

We note that, although Φ is completely antisymmetric for the interchange of any pair of particles, it is a function of the internal spatial coordinates only of the $(A+1)$ -particles.

We now consider the matrix element of Φ_r with another general state χ_s of the A -particle nucleus. For convenience we take it in a coupled form using a generalized angular function defined by eq. (9)

$$M(sj', rj; |\mathbf{r}_{A+1} - \mathbf{B}_A|) = \langle [\chi_s(1 \dots A; J_s T_s T_{3s}) \phi(\Omega_{A+1} \mathbf{r}_{A+1} \mathbf{r}_{A+1}; j' l' t_3')]_M^J, \Phi_r \rangle \quad (17)$$

where Ω_{A+1} refers to the variable $\mathbf{r}_{A+1} - \mathbf{B}_A$.

The evaluation of this matrix element in two different ways forms the basis of our technique.

Firstly we insert the unit operation $\mathbb{I}_{A+1}$, given by eq. (2), for the $(A+1)$ -particle Hamiltonian and use the coupled overlap definition (11).

$$\begin{aligned} M(sj', rj; |\mathbf{r}_{A+1} - \mathbf{B}_A|) &= \sum_{n, J_n = J} \theta'_{sn}(j' l' t_3') \theta'_{rn}(j l' t_3') \\ &\langle \phi_{rn}(j l t_3), \phi(j l t_3) \rangle \phi_{sn}(|\mathbf{r}_{A+1} - \mathbf{B}_A|; j' l' t_3') \\ &+ \sum_n \int d^3 \mathbf{B}_n (A+1) \langle [\chi_s \phi(\Omega_{A+1})]_M^J, \Psi_n^{(+) }(\mathbf{B}_n) \rangle \\ &\langle \Psi_n^{(+) }(\mathbf{B}_n), [\chi_r \phi(A+1)]_M^J \rangle \end{aligned} \quad (18)$$

The full quantal labelling of the final continuum term is defined above. In this paper we shall not consider its further evaluation or detailed properties but merely define it to be $M_c(s_j', r_j, J; |x_{A+1} - B_A|)$.

Secondly, we may evaluate M directly using the definition (16). Clearly all the permutation operators are equivalent and we obtain

$$M(s_j', r_j; |x_{A+1} - B_A|) = \Phi(|x_{A+1} - B_A|; j \ell t_3)$$

$$S_{rs} S_{jj'} S_{\ell\ell'} S_{t_3 t_3'} = \Lambda(s_j', r_j; |x_{A+1} - B_A|) \quad (19)$$

where the exchange term is

$$\Lambda(s_j', r_j; |x_{A+1} - B_A|) = A < [X_s(1 \dots A-1, x_A - B_{A-1}, \varpi_A, \Xi_A;$$

$$J_s T_s T_{3s}) \Phi(\Omega_{x_{A+1} - B_A}, \varpi_{A+1}, \Xi_{A+1}; j' \ell' t_3') \Big]_M^J,$$

$$[X_r(1 \dots A-1; x_{A+1} - B_{A-1}, \varpi_{A+1}, \Xi_{A+1}; J_r T_r T_{3r})$$

$$\Phi(x_A - \frac{1}{A} x_{A+1} - \frac{1}{A} \sum_{i=1}^{A-1} x_i, \varpi_A, \Xi_A; j \ell t_3) \Big]_M^J > \quad (20)$$

The dependence on the co-ordinates, x_A and x_{A+1} has been shown in full.

It is convenient to redefine two variables as

$$x = x_{A+1} - B_A, \quad \varpi = x_A - B_{A-1} \quad (21)$$

In terms of these variables with some quantum numbers suppressed we have, using Taylor expansions,

$$\begin{aligned}
 \Lambda(s, j', r, j; r) &= A \left\langle \left[\chi_s(1 \dots A-1, \underline{x}; J_s) \phi(\Omega_{\underline{x}}; j') \right]_M^J, \right. \\
 &\left. \left[\chi_r(1 \dots A-1, \underline{r} + \frac{1}{A} \underline{x}; J_r) \phi\left(\left(1 - \frac{1}{A^2}\right) \underline{x} - \frac{1}{A} \underline{r}; j\right) \right]_M^J \right\rangle \\
 &= A \left\langle \left[\chi_s(1 \dots A-1, \underline{x}; J_s) \phi(\Omega_{\underline{x}}; j') \right]_M^J \left[1 + \frac{1}{A} (\underline{x} \cdot \nabla_{\underline{r}} - \underline{r} \cdot \nabla_{\underline{x}}) \right] \right. \\
 &\left. \left[\chi_r(1 \dots A-1, \underline{r}; J_r) \phi(\Omega_{\underline{r}}; j) \right]_M^J + O(1/A^2) \right\rangle. \quad (22)
 \end{aligned}$$

The correction term of order $1/A$ is evaluated in sect. 5. To evaluate the first term we introduce a coupled unit operator for the $(A-1)$ -particle Hamiltonian obtained from I_{A-1} given by eq. (1) in terms of the states

$$\left[\left[\Psi_{\alpha}(1 \dots A-1; J_{\alpha} T_{\alpha} T_{3\alpha}) \phi(\Omega_{\underline{x}}; j, t_3) \right]^{J_s} \phi(\Omega_{\underline{r}}; j', t_3') \right]_M^J$$

Evidently the quantum numbers in the variables $\underline{x}$ and $\underline{r}$ are fixed so the summation only runs over α . The evaluation of the left hand matrix element immediately follows from definition (10). To evaluate the right hand matrix element we recouple Ψ_{α} to $\phi(\Omega_{\underline{x}})$ and use the same definition. The result is

$$\Lambda(sj', rj; r) = \sum_{\alpha} (-1)^{J_r + J_s + j + j'} [(2J_r + 1)(2J_s + 1)]^{1/2}$$

$$\left\{ \begin{matrix} J_r & j & J_r \\ J_{\alpha} & j' & J_s \end{matrix} \right\} \Theta'_{\alpha s}(j l t_3) \Theta'_{\alpha r}(j' l' t'_3)$$

$$\langle \phi_{\alpha s}(j l t_3), \phi(j l t_3) \rangle \phi_{\alpha r}(r; j' l' t'_3) \quad (23)$$

From eqs. (18), (19) and (23) we can write the relation, exact to zero order in $1/A$, as

$$\phi(r; j l t_3) \delta_{rs} \delta_{jj'} \delta_{ll'} \delta_{t_3 t'_3} = \sum_{n, J_n \text{ fixed}} \Theta'_{sn}(j' l' t'_3)$$

$$\Theta'_{rn}(j l t_3) \langle \phi_{rn}, \phi \rangle \phi_{sn}(r; j' l' t'_3)$$

$$+ \sum_{\alpha} (-1)^{J_r + J_s + j + j'} [(2J_r + 1)(2J_s + 1)]^{1/2} \left\{ \begin{matrix} J_n & j & J_r \\ J_{\alpha} & j' & J_s \end{matrix} \right\}$$

$$\Theta'_{\alpha s}(j l t_3) \Theta'_{\alpha r}(j' l' t'_3) \langle \phi_{\alpha s}, \phi \rangle \phi_{\alpha r}(r; j' l' t'_3)$$

$$+ M_c(sj', rj, J_n; r) \quad (24)$$

These equations may be put in an alternative form, in which the roles of the particles removed and added are interchanged, by applying

the operation

$$\sum_{J_n} (-1)^{J_r + J_s + j + j'} (2J_n + 1) \left\{ \begin{matrix} J_n & j & J_r \\ J_{\alpha'} & j' & J_s \end{matrix} \right\}.$$

Then

$$\begin{aligned} & \phi(r; j \ell t_3) \delta_{rs} \delta_{jj'} \delta_{\ell \ell'} \delta_{t_3 t_3'} \\ &= \sum_{\alpha, J_{\alpha} \text{ fixed}} \frac{[(2J_r + 1)(2J_s + 1)]^{1/2}}{(2J_{\alpha} + 1)} \theta'_{\alpha s}(j \ell t_3) \theta'_{\alpha r}(j' \ell' t_3') \\ & < \phi_{\alpha s}, \phi > \phi_{\alpha r}(r; j' \ell' t_3') + \sum_n (2J_n + 1) (-1)^{J_r + J_s + j + j'} \\ & \left\{ \begin{matrix} J_n & j & J_r \\ J_{\alpha} & j' & J_s \end{matrix} \right\} \theta'_{s n}(j' \ell' t_3') \theta'_{r n}(j \ell t_3) < \phi_{r n}, \phi > \\ & \phi_{s n}(r; j' \ell' t_3') + \sum_{J_n} (-1)^{J_r + J_s + j + j'} (2J_n + 1) \\ & \left\{ \begin{matrix} J_n & j & J_r \\ J_{\alpha} & j' & J_s \end{matrix} \right\} M_c(s j', r j, J_n; r) \end{aligned} \quad (25)$$

where we have used the orthogonality property of the 6-j symbols and the special result

$$\sum_J (-1)^{2j + 2J_r} (2J + 1) \left\{ \begin{matrix} j & J_r & J_{\alpha} \\ j & J_r & J \end{matrix} \right\} = 1 \quad (26)$$

The alternative sets of equations (24) or (25) embody the principal results of this work. In relation to the more usual concepts of nuclear

physics we may ask what is their physical content? For the diagonal equation the answer was partly provided in ref. 5) where it was shown that, if the continuum contribution is neglected, the $\phi_{\alpha r}$ and ϕ_{rn} are not linearly independent and can be expressed in terms of underlying single particle states, χ_λ . The χ_λ may be characterised by principal quantum numbers and can be identified as the shell model single particle wave functions for the nucleus in question. It is intuitively obvious, though this has not been rigorously proved, that the inclusion of the continuum states will mix in small continuum components (corresponding to higher harmonic oscillator principal quantum numbers in the shell model) to give the actual physical overlap functions. The extent of this continuum mixing is a subject for further research.

The above equations immediately generalise these results for a nucleus with non-zero spin and for excited states of the A-particle nucleus. However, for highly excited states one might expect considerable continuum mixing. Otherwise one expects the χ_λ to be almost identical for different states of the A-particle nucleus. This non-independence is reflected in the off-diagonal equations with $r \neq s$ and identical single particle quantum numbers, $j \ell t_3$, which then become effective orthogonality relations between the single particle density matrices of different states. For example, with $\phi \equiv \chi_\lambda(j \ell t_3) \approx \phi_{rn} \approx \phi_{sn} \approx \phi_{\alpha r} \approx \phi_{\alpha s}$, we have from eq. (24)

$$\sum_{n, J_n \text{ fixed}} \theta'_{sn} \theta'_{rn} + \sum_{\alpha} (-1)^{J_r + J_s + 1} [(2J_r + 1)(2J_s + 1)]^{1/2}$$

$$\left\{ \begin{matrix} J_n & j & J_r \\ J_n & j & J_s \end{matrix} \right\} \theta'_{\alpha s} \theta'_{\alpha r} = 0 \quad (27)$$

where M_c has been neglected.

All the other off-diagonal equations are also effective orthogonality relations. For the interesting case of $r=s$, $J_r \neq 0$ and $j \neq j'$, eq. (25) becomes approximately

$$\sum_{\alpha, J_\alpha \text{ fixed}} \frac{(2J_r+1)}{(2J_\alpha+1)} \Theta'_{\alpha r}(j) \Theta'_{\alpha r}(j') + \sum_n (2J_n+1) (-1)^{2J_r+j+j'} \left\{ \begin{matrix} J_n & j & J_r \\ J_\alpha & j' & J_r \end{matrix} \right\} \Theta'_{rn}(j') \Theta'_{rn}(j) = 0. \quad (28)$$

All the off-diagonal equations should have shell model counterparts though, to our knowledge, these have not been derived. They may well have uses in constructing models for excited states of nuclei such as 'particle-hole' models but we shall not pursue the subject here. However, we wish to note the equations which apply whenever a shell is entirely open or completely closed.

In our context a shell, $j \leq t_3$, is open for state r when represented by a wave function $\phi \equiv \chi_\lambda(j \leq t_3)$ such that

$$\langle \chi_\lambda, \phi_{\alpha r} \rangle \approx 0, \quad \text{for all } \alpha. \quad (29)$$

Similarly it is completely closed if

$$\langle \chi_\lambda, \phi_{rn} \rangle \approx 0, \quad \text{for all } n \quad (30)$$

and the continuum contribution is negligible.

For an open $(j\ell t_3)$ -shell in state s , we have, from eq. (27),

$$\sum_{n, J_n \text{ fixed}} \Theta'_{sn}(j'\ell' t_3') \Theta'_{rn}(j\ell t_3) \approx 0 \quad (31)$$

If the $(j\ell t_3)$ -shell is closed in state r , from eq. (28) we get

$$\sum_{\alpha, J_\alpha \text{ fixed}} \Theta'_{\alpha s}(j\ell t_3) \Theta'_{\alpha r}(j'\ell' t_3') \approx 0 \quad (32)$$

We note that, for example in the latter relation, the shell may not be closed in s and there is no restriction on the shell $j'\ell' t_3'$ except, of course, that it is not identical to $j\ell t_3$ for $r=s$.

We now turn to a detailed consideration of the diagonal equations and the exact sum rules to be derived from them.

4. Partial Sum Rules.

Exact sum rules giving the distribution of any normalized function $\phi(r, j, t_3)$ over the overlap functions can be obtained from either of the diagonal eqs. (24) or (25) by multiplying by ϕ and integrating over r . From eq. (24) we obtain

$$\begin{aligned}
 1 &= \sum_{n, J_n \text{ fixed}} S'_{rn}(j, t_3) |\langle \phi_{rn}, \phi \rangle|^2 \\
 &+ \sum_{\alpha} (-1)^{2J_r+1} (2J_r+1) \left\{ \begin{matrix} J_n & j & J_r \\ J_\alpha & j & J_r \end{matrix} \right\} S'_{\alpha r}(j, t_3) \\
 |\langle \phi_{\alpha r}, \phi \rangle|^2 &+ S_{rc}(j, t_3, J_n),
 \end{aligned} \tag{33}$$

where the continuum contribution is defined as

$$S_{rc}(j, t_3, J_n) = \int dr \, r^2 \phi(r) M_c(rj, rj, J_n; r). \tag{34}$$

Similarly eq. (25) gives

$$\begin{aligned}
 1 &= \frac{2J_r+1}{2J_\alpha+1} \sum_{\alpha, J_\alpha \text{ fixed}} S'_{\alpha r}(j, t_3) |\langle \phi_{\alpha r}, \phi \rangle|^2 \\
 &+ \sum_{J_n} (2J_n+1) (-1)^{2J_r+1} \left\{ \begin{matrix} J_n & j & J_r \\ J_\alpha & j & J_r \end{matrix} \right\} \left[\sum_{n, J_n \text{ fixed}} S'_{rn}(j, t_3) \right. \\
 &\left. |\langle \phi_{rn}, \phi \rangle|^2 + S_{rc}(j, t_3, J_n) \right].
 \end{aligned} \tag{35}$$

The quantities $S'_{\alpha r}$ and $[(2J_n+1)S'_{rn}/(2J_r+1)]$ are those extracted directly from an analysis of experimental stripping and pickup reactions, particularly when the spin J_n is unknown. We therefore define the following partial sums for stripping and pickup reactions, respectively, where the explicit dependence on j, l, t_3, r and ϕ is dropped,

$$S_{J_n}^+ = \frac{2J_n+1}{2J_r+1} \sum_{n, J_n \text{ fixed}} S'_{rn} |\langle \phi_{rn}, \phi \rangle|^2$$

$$S_{J_\alpha}^- = \sum_{\alpha, J_\alpha \text{ fixed}} S'_{\alpha r} |\langle \phi_{\alpha r}, \phi \rangle|^2$$

$$S_{cJ_n} = \frac{2J_n+1}{2J_r+1} S_{rc}(J_n) \quad (36)$$

In terms of these partial sums the sum rules become

$$\frac{2J_n+1}{2J_r+1} = S_{J_n}^+ + S_{cJ_n} + (2J_n+1)(-1)^{2J_r+1} \sum_{J_\alpha} \left\{ \begin{matrix} J_\alpha & j & J_r \\ J_n & j & J_r \end{matrix} \right\} S_{J_\alpha}^- \quad (37)$$

$$\frac{2J_\alpha+1}{2J_r+1} = S_{J_\alpha}^- + (2J_\alpha+1)(-1)^{2J_r+1} \sum_{J_n} \left\{ \begin{matrix} J_n & j & J_r \\ J_\alpha & j & J_r \end{matrix} \right\} (S_{J_n}^+ + S_{cJ_n}) \quad (38)$$

These sets of equations may be transformed into each other using the orthogonality of the 6-j symbols. The summation of the first over J_n

or the second over J_α and use of eq. (26) gives the total sum rule

$$\sum_{J_n} (S_{J_n}^+ + S_{cJ_n}) + \sum_{J_\alpha} S_{J_\alpha}^- = 2j + 1. \quad (39)$$

If $J_r=0$ there is only one sum rule which was obtained previously.^{3,4)}

If all the ϕ_s are equal and the continuum contribution is neglected, the sum rules (37) and (36) become the shell model sum rules derived by French⁸⁾. In spite of their potential usefulness in nuclear physics repeatedly pointed out by French, very few applications of them have been made hitherto. P. Hodgson¹⁸⁾ has applied them to $\ell = 1$ transitions on ^{57}Fe with encouraging results. This mainly arises from large gaps in experimental data for one-nucleon transfer reactions on odd-mass nuclei. It therefore seems worthwhile to emphasize some of their possible applications.

(a) $\ell = 0$ Transfer.

This is a particularly favourable case as pointed out by French⁸⁾ since only $j = 1/2$ transfer is involved and there is no ambiguity in assigning the j -value. In this case the two linear equations may be written in the form

$$S_{J_r + \frac{1}{2}}^+ = \frac{1}{2J_r + 1} \left[2(J_r + 1) - \frac{n}{r_1 + 1} (2r_1(J_r + 1) + 1) \right]$$

$$S_{J_r - \frac{1}{2}}^+ = \frac{1}{2J_r + 1} \left[2J_r - \frac{n}{r_1 + 1} (2J_r - r_1) \right], \quad (40)$$

where

$$S_{J_+ + 1/2}^- + S_{J_+ - 1/2}^- = n, \quad S_{J_+ - 1/2}^- / S_{J_+ + 1/2}^- = r_1 \quad (41)$$

Here, n is the occupancy of the shell, ranging in value between 0 and 2. The equations may be written in a similar form for the pickup spectroscopic sums S^+ . From the requirement that the S^+ are positive we find the restriction on r_1 , given n ,

$$\frac{2J_+(n-1)}{2J_+ + n} \leq r_1 \leq \frac{1}{2(J_+ + 1)} \frac{2(J_+ + 1) - n}{(n-1)} \quad (42)$$

There is a similar restriction for $r_2 = S_{J_+ - 1/2}^+ / S_{J_+ + 1/2}^+$ with n replaced by $2-n$. In a plot of n against r_1 or r_2 there are excluded regions as shown in Fig. 1. If the shell is nearly empty or nearly full the value of one of the ratios is very strongly restricted.

Comparison with experiment in the $1d\ 2s$ shell is hampered at present by lack of data. Relative spectroscopic factors obtained from Butler theory for $\ell = 0$ transitions are quoted for the reaction $^{27}\text{Al} (d-p)^{28}\text{Al}$.¹⁹⁾ If the $2s\ 1/2$ neutron shell were empty in ^{27}Al we would have a unique ratio, $r_2 = S_2^+ / S_3^+ = 5/7$. For the lowest two final states, whose spins are established as 3^+ and 2^+ we have $r_2 = 0.53$ which gives an occupancy $n \geq 0.29$. If the 2.143 MeV state, which has most of the remaining $\ell = 0$ strength, has spin 3^+ , $r_2 = 0.4$ giving $n \geq 0.48$. If it has spin 2^+ we have $r_2 = 0.87$ which leads to $n \geq 0.13$. According to Lawergren²⁰⁾, who obtained absolute spectroscopic factors through the $2s\ 1/2$ shell, $n \approx 0.3$ which would be

inconsistent with a 3^+ spin assignment. This discussion points to the usefulness of the partial sum rules in aiding spin assignments, an application we now consider in more detail.

(b) Spin Assignments and the $1f_{7/2}$ Shell.

Because there is likely to be little mixing of $1f_{5/2}$ strength into low-lying states with $\Delta = 3$ transitions, the $1f_{7/2}$ shell is potentially one of the best areas of application of the sum rules. The sum rules should be a powerful aid in making spin assignments.

Let us consider a possible application to the nucleus ^{45}Sc for which $J_r = 7/2$. The stripping and pickup of an $f_{7/2}$ neutron should lead mainly to low-lying states in the final nucleus with spins ranging between 0 and 7. The sum rules thus give 8 linear equations between 16 sums of spectroscopic factors. From an examination of existing data it is apparent that most of the strength for a given spin is generally concentrated in a single state. In addition, realistically we should allow for a possible error in the absolute value of the spectroscopic factors for stripping and pickup. This increases the number of parameters to 18 or 17 if we insist that the total sum rule (39) is satisfied and neglect any continuum contribution.

Experimentally the (p,d) reaction to ^{44}Sc has been performed up to an excitation energy of about 1 MeV by Kashy²¹⁾. Some spin assignments have been made on the basis of the $^{43}\text{Ca}(\text{He}^3\text{-d})^{44}\text{Sc}$ reaction by Schwartz²²⁾. Incidentally it can be seen that some of the theoretical values for the spectroscopic factors based on an $(f_{7/2})^4$ configuration which are quoted in this paper do not satisfy the partial sum rules.

Unfortunately the (p,d) reaction has not covered the energy region for all the $f_{7/2}$ strength and in particular the 0^+ state, which can only be reached by $f_{7/2}$ transfer is not included. It would therefore, be highly desirable to perform a neutron pickup reaction on ^{45}Sc to higher excited states.

The reaction $^{45}\text{Sc}(d,p)^{46}\text{Sc}$ has been performed by Rapaport et. al.²³⁾ up to an energy which should include most of the $f_{7/2}$ strength. Several spin assignments have been made by Lewis²⁴⁾ using the $^{48}\text{Ti}(d,\alpha)^{46}\text{Sc}$ reaction. The present situation is that there are about 3 definite spin assignments for each nucleus with several others suggested.

Because of absolute magnitude uncertainties, missing strength to 0^+ and possibly other spin states no detailed analysis has yet been attempted on the basis of the sum rules. A sophisticated numerical method is definitely required as use of the equations as they stand with some spins known in each nucleus is clearly inadequate. However, one can check on the basis of likely assignments for ^{46}Sc that $S_6^- + S_7^- \approx 1.7$ with a possible negative error. The spectroscopic factors for the 271 keV and 952 keV states in ^{44}Sc are 0.47 and 1.36, respectively, and the former is definitely established as 6^+ . Their sum of ≈ 1.8 serves to confirm Schwartz's assignment²²⁾ of 7^+ to the 952 keV states.

In conclusion $f_{7/2}$ transitions on ^{45}Sc with a little more data should serve as one of the best tests of the sum rules in the periodic table and it may be possible to make more definite spin assignments for ^{44}Sc and ^{46}Sc .

5. Centre of Mass Corrections.

In this section we obtain, to order $1/A$, corrections to the principal results obtained hitherto. Corrections are found to occur for a given $(j\ell)$ sum rule when single particle states $(j_1\ell_1)$ connected to $(j\ell)$ by a dipole operator are occupied. The general formulae are simplified in two cases. Firstly, when $(j_1\ell_1)$ is completely occupied, which is generally the case when $(j\ell)$ is a valence level, we give the corrections for the partial and total sum rules. Secondly, the correction for the total sum rule is obtained in the general case.

The formulae obtained here are evaluated using simple Harmonic oscillator wave functions in the next section where detailed sum rule corrections for light nuclei are discussed.

From eq. (22) the $1/A$ correction to the exchange term Λ is

$$\Lambda_1(sj', rj; r) = \langle [\chi_s(1 \dots A-1, \underline{x}; J_s) \phi(\Omega_{\underline{x}}; j')]]_M^J, \\ (\underline{x} \cdot \nabla_{\underline{x}} - \underline{x}' \cdot \nabla_{\underline{x}'}), [\chi_r(1 \dots A-1, r; J_r) \phi(\Omega_{\underline{x}}; j)]]_M^J \rangle \quad (43)$$

The initial and final wave functions are expanded in the following coupled complete sets obtained from the unit operator I_{A-1} , given by eq. (1);

$$[[\Psi_{\alpha}(1 \dots A-1, J_{\alpha}) \phi(\Omega_{\underline{x}}; j_1)]]^{J_r} \phi(\Omega_{\underline{x}}; j)]_M^J$$

and

$$[[\Psi_{\alpha}(1 \dots A-1, J_{\alpha}) \phi(\Omega_{\underline{x}}; j_2)]]^{J_s} \phi(\Omega_{\underline{x}}; j')]_M^J$$

where the omitted quantum numbers are labelled similarly and the summation runs over α , j_1 and j_2 .

From the definition (10) and one recoupling we obtain

$$\Lambda_1(s, j', r, j; r) = \frac{1}{A} \sum_{\alpha, j_1, l_1, j_2, l_2} \Theta'_{\alpha s}(j_2, l_2, t_3) \Theta'_{\alpha r}(j_1, l_1, t_3')$$

$$\sum_{J_s'} (-1)^{j_1 + j + J_r + J_s'} \left[(2J_r + 1)(2J_s' + 1) \right]^{1/2} \left\{ \begin{matrix} J_\alpha & j_1 & J_r \\ J & j & J_s' \end{matrix} \right\}$$

$$\left\langle \left[\left[\Psi_\alpha(1 \dots A-1; J_\alpha) \phi_{\alpha s}(\underline{x}, \underline{x}_A; j_2 l_2) \right]^{J_s} \phi(\underline{\Omega}_\alpha, \underline{x}_{A+1}; j' l') \right]_m^{J_s} \right\rangle$$

$$(\underline{x} \cdot \nabla_{\underline{x}} - \underline{x}' \cdot \nabla_{\underline{x}'}), \left[\left[\Psi_\alpha(1 \dots A-1; J_\alpha) \phi(\underline{x}, \underline{x}_A; j l) \right]^{J_s} \right]$$

$$\phi_{\alpha r}(\underline{x}, \underline{x}_{A+1}; j_1 l_1) \Big]_m^{J_s} > .$$

The matrix element can now be evaluated by standard methods in terms of reduced matrix elements and the sum over J_s' performed to give

$$\Lambda_1(s, j', r, j; r) = \frac{1}{A} \sum_{\alpha, j_1, l_1, j_2, l_2} \Theta'_{\alpha s}(j_2, l_2, t_3) \Theta'_{\alpha r}(j_1, l_1, t_3')$$

$$(-1)^{j_1 + j' + J_\alpha + J_r + J_s + J} \left[(2J_r + 1)(2J_s + 1) \right]^{1/2} \left\{ \begin{matrix} J_\alpha & J_s & j_2 \\ j_1 & j' & 1 \\ J_r & J & j \end{matrix} \right\}$$

$$\left[M_1 M_2(r) - M_2 M_1(r) \right], \quad (44)$$

where the reduced matrix elements are

$$\begin{aligned}
 M_1 &= \langle \phi_{\alpha s}(\underline{x}, \underline{\sigma}_A; j_2 l_2) \| \underline{x} \| \phi(\underline{x}, \underline{\sigma}_A; j l) \rangle \\
 &= \delta_{l_2 l+1} (-1)^{j_2 + \frac{1}{2}} [(2j+1)(2j_2+1)]^{\frac{1}{2}} \begin{pmatrix} j_2 & 1 & j \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} \\
 &\quad \int dx x^3 \phi_{\alpha s}(x; j_2 l_2) \phi(x; j l), \quad (45a)
 \end{aligned}$$

$$\begin{aligned}
 M_1(r) &= \langle \phi(\Omega \underline{x}, \underline{\sigma}_{A+1}; j' l') \| \underline{x} \| \phi_{\alpha r}(\underline{x}, \underline{\sigma}_{A+1}; j_1 l_1) \rangle \\
 &= \delta_{l_1 l'+1} (-1)^{j_1 + \frac{1}{2}} [(2j'+1)(2j_1+1)]^{\frac{1}{2}} \begin{pmatrix} j' & 1 & j_1 \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} \\
 &\quad + \phi_{\alpha r}(r; j_1 l_1), \quad (45b)
 \end{aligned}$$

$$\begin{aligned}
 M_2 &= \langle \phi_{\alpha s}(\underline{x}, \underline{\sigma}_A; j_2 l_2) \| \nabla_{\underline{x}} \| \phi(\underline{x}, \underline{\sigma}_A; j l) \rangle \\
 &= (-1)^{j+l} \delta_{l_2 l-1} [(2j+1)(2j_2+1) l_2]^{\frac{1}{2}} \begin{Bmatrix} l_2 & l & 1 \\ j & j_2 & \frac{1}{2} \end{Bmatrix} \\
 &\quad \int dx x^2 \phi_{\alpha s}(x; j_2 l_2) \begin{cases} \frac{\partial}{\partial x} - \frac{l}{x} \\ \frac{\partial}{\partial x} + \frac{l+1}{x} \end{cases} \phi(x; j l), \quad \begin{matrix} l_2 = l+1 \\ l_2 = l-1 \end{matrix} \\
 &\quad (45c)
 \end{aligned}$$

$$\begin{aligned}
 M_2(r) &= \langle \phi(\Omega \underline{x}, \underline{\sigma}_{A+1}; j' l') \| \nabla_{\underline{x}} \| \phi_{\alpha r}(\underline{x}, \underline{\sigma}_{A+1}; j_1 l_1) \rangle \\
 &= (-1)^{j_1+l} \delta_{l_1 l-1} [(2j'+1)(2j_1+1) l_1]^{\frac{1}{2}} \begin{Bmatrix} l' & l_1 & 1 \\ j_1 & j' & \frac{1}{2} \end{Bmatrix} \\
 &\quad \begin{cases} \frac{\partial}{\partial r} - \frac{l_1}{r} \\ \frac{\partial}{\partial r} + \frac{l_1+1}{r} \end{cases} \phi_{\alpha r}(r; j_1 l_1), \quad \begin{matrix} l' = l_1+1 \\ l' = l_1-1 \end{matrix} \quad (45d)
 \end{aligned}$$

where $\ell_>$ refers to the larger of the two ℓ values involved and the appropriate derivative operator corresponding to the ℓ values given is to be taken.

The $1/A$ correction, $\Lambda_1(sj', rj; r)$ with $J = J_n$ should be added to the right hand side of eq. (24). We note that it involves occupied orbits ℓ_1, ℓ_2 of opposite parity and differing by one unit of orbital angular momentum from ℓ' and ℓ respectively.

The result (44) is perfectly general but let us immediately go on to consider the corrections to the sum rules obtained by multiplying by $r^2 \phi(r; j\ell')$ and integrating over r . We will find in our two special cases, which cover almost all situations of physical interest, that there are only corrections to the diagonal sum rules where $(j'\ell') = (j\ell)$.

First we consider the case when either of $(j_1\ell_1)$ or $(j_2\ell_2)$ shells is fully occupied in r or s , respectively, or, in other words, closed in the sense of the discussion of section 3. If we then neglect any dependence of M_1 or M_2 on α , an approximation expected to be very good and consistent with the 'closed shell' approximation, we can make use of eq. (32). The summation over α for fixed J_α in Λ_1 given by the integrated eq. (44) then vanishes unless $j_1\ell_1 t_3' + j_2\ell_2 t_3 = 0$. Furthermore, since $(j_1\ell_1)$ is closed we have from eqs. (36) and (38),

$$\sum_{\alpha, J_\alpha \text{ fixed}} S'_{\alpha r}(j_1\ell_1 t_3) \approx \frac{2J_\alpha + 1}{2J_r + 1}$$

For a given $(j_1\ell_1 t_3)$ the sum over J_α in eq. (44) now takes the form

$$\sum_{J_z} (-1)^{j_1 + j' + 2J_z + J + J_z} (2J_z + 1) \begin{Bmatrix} J_z & J_z & j_1 \\ j_1 & j' & 1 \\ J_z & J & j \end{Bmatrix}$$

$$= \frac{(-1)^{j_1 + j + 1}}{2j + 1} \delta_{jj'} \quad (46)$$

The requirement that $\ell = \ell'$ now follows from $j = j'$, $\ell_1 = \ell_2$ and the nature of the dipole matrix elements. Thus our first conclusion is that, when all the allowed $(j_1 \ell_1)$ or $(j_2 \ell_2)$ are closed, the off-diagonal sum rules or orthogonality relations have no correction to order $1/A$.

On the other hand the diagonal sum rules have a correction. Since $(j' \ell') = (j \ell)$ and we choose $\phi(r; j' \ell')$ to have the same radial form as $\phi(r; j \ell)$, the two integrated terms in Λ_1 are equal because of the anti-Hermitian nature of the ∇ operator. From eqs. (44), (45) and (46) the correction is

$$\Delta_1(j \ell \ell_3) = \frac{2}{A} \sum_{j_1 \ell_1} \frac{(-1)^{j_1 + j + 1}}{2j + 1} \langle \psi(j_1 \ell_1) || \underline{x} || \phi(j \ell) \rangle$$

$$\langle \phi(j \ell) || \nabla_{\underline{x}} || \psi(j_1 \ell_1) \rangle, \quad (47)$$

where all the $\phi_{\alpha r}(\underline{x}; j_1 \ell_1)$ have been replaced by the closed shell overlap function $\psi(\underline{x}; j_1 \ell_1)$.

This quantity should be added to the right hand side of eq. (33) so that the sum rules (37) and (39) become

$$\frac{2J_n + 1}{2J_r + 1} (1 - \Delta_1) = S_{J_n}^+ + S_{cJ_n} + (2J_n + 1)(-1)^{2J_r+1} \sum_{J_\alpha} \left\{ \begin{matrix} J_\alpha & j & J_r \\ J_n & j & J_r \end{matrix} \right\} S_{J_\alpha}^- \quad (48)$$

and

$$\sum_{J_n} (S_{J_n}^+ + S_{cJ_n}) + \sum_{J_\alpha} S_{J_\alpha}^- = (2j+1)(1 - \Delta_1). \quad (49)$$

The modification of sum rule (38) follows from eq. (48) since Δ_1 is independent of J_n .

Before proceeding to the second case we anticipate our finding that if $(j\ell)$ is a valence level and $(j_1\ell_1)$ is an occupied level, Δ is negative so that the sum rules of experimental quantities should take on larger values than previously.

To obtain the general correction to the total sum rule (39) we take $(j\ell t_3 r) = (j'\ell' t_3' s)$ in eq. (44) and integrate over r with $r^{-2} \phi(r; j\ell)$. The correction is then found by multiplying by $(2J_n+1)/(2J_r+1)$ and summing over J_n . Since M_1 and M_2 are independent of J_n , the latter sum takes a similar form to eq. (46) and contains $S_{j_1 j_2}$. Again from the dipole matrix elements we have $\ell_1 = \ell_2$ so that the total sum rule takes the form (49) with the exact $1/A$ correction

$$(2j+1) \Delta_1(j\ell t_3) = \frac{1}{A} \sum_{j_1 \ell_1} \frac{(-1)^{j_1+j+1}}{2j_1+1} S'_{\alpha r}(j_1 \ell_1 t_3) \int dr r^{-2} \phi(r; j\ell) [M_1 M_2(r) - M_2 M_1(r)], \quad (50)$$

where M_1 and M_2 are given by eq. (45) with $(j\ell + j_1\ell_1) = (j'\ell' + j_2\ell_2)$.

If we take all the $\phi_{\alpha+}(\underline{x}; j_1\ell_1)$ to be identical to a shell model overlap function, $\psi(\underline{x}; j_1\ell_1)$, we obtain the following generalization of eq. (47);

$$(2j+1) \Delta_1(j\ell t_3) = \frac{2}{A} \sum_{j_1\ell_1} (-1)^{j_1+j+1} \left[\sum_{\alpha} \frac{S'_{\alpha+}(j_1\ell_1 t_3)}{2j_1+1} \right]$$

$$\langle \psi(j_1\ell_1) || \underline{x} || \phi(j\ell) \rangle \langle \phi(j\ell) || \nabla_{\underline{x}} || \psi(j_1\ell_1) \rangle$$

(51)

This expression reduces to (47) when shell $(j_1\ell_1)$ is full and the sum over α is unity to lowest order in $1/A$.

6. Sum Rule Corrections for Light Nuclei.

We now proceed to evaluate the sum rule corrections (47) and (51) using a simple model and then discuss some applications to light nuclei. It would clearly be possible to evaluate the correction (50) using realistic overlap functions and the expressions (45). However, this would have to be done numerically and, as the overall correction is small anyway, estimates based on shell-model wave functions should be accurate enough for most purposes.

We assume that ψ , ϕ in the matrix elements of eqs. (47) and (51) are defined by some local shell model potential contained in $H_{s.p.}$ so that

$$H_{s.p.} \phi(j\ell) = E_{j\ell} \phi(j\ell), \quad H_{s.p.} \psi(j_1\ell_1) = E_{j_1\ell_1} \psi(j_1\ell_1)$$

and

$$-\frac{\hbar^2}{M} \nabla_{\vec{x}} = [H_{s.p.}, \vec{x}].$$

The commutator replaces the matrix element of $\nabla_{\vec{x}}$ in eq. (51) by that of $M/\hbar^2 (E_{j_1\ell_1} - E_{j\ell}) \vec{x}$ so that, using eq. (45a) we obtain

$$(2j+1) \Delta_1(j\ell t_3) = \frac{2M}{\hbar^2} (2j+1) \sum_{j_1\ell_1} S_{\ell_1\ell+1} S^-(j_1\ell_1 t_3) \\ \left(\begin{array}{ccc} j_1 & 1 & j \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{array} \right)^2 D^2(j\ell; j_1\ell_1) (E_{j_1\ell_1} - E_{j\ell}), \quad (52)$$

where the radial dipole integrals are defined by

$$D(j\ell; j_1 \ell_1) = \int dx x^3 \phi(x; j\ell) \psi(x; j_1 \ell_1) \quad (53)$$

and

$$S^-(j_1 \ell_1 t_3) = \sum_{\alpha} S'_{\alpha+}(j_1 \ell_1 t_3). \quad (54)$$

Now we specialize further to take ϕ and ψ as Harmonic oscillator wave functions defined by the principal quantum numbers n and n_1 , respectively. (n = number of nodes, i.e., $n = 0$ for $1s1/2$ state).

$$D^2(nj\ell; n_1 j_1 \ell_1) = \frac{2n + 2\ell + 3}{4\nu} S_{nn_1} + \frac{n+1}{2\nu} S_{n_1 n+1} \delta_{\ell_1 \ell-1} + \frac{n_1+1}{2\nu} S_{nn_1+1} \delta_{\ell \ell_1-1}, \quad (55)$$

where $\nu = M\omega/2\hbar$.

To the degree of approximation needed we can take the energy difference to be given by the oscillator energy difference with the sign given formally by

$$E_{j_1 \ell_1} - E_{j\ell} = \hbar\omega \left[\delta_{n_1 n} (\delta_{\ell, \ell+1} - \delta_{\ell \ell-1}) + \delta_{n_1 n+1} \delta_{\ell_1 \ell-1} - \delta_{nn_1+1} \delta_{\ell \ell_1-1} \right] \quad (56)$$

Thus Δ_1 is negative for corrections arising from an occupied lower major shell and positive for those from an occupied higher shell. From eqs. (52) (54), (55) and (56) we rewrite the sum rule (49) as

$$\begin{aligned} \sum_{J_n} (S_{J_n}^+ + S_{cJ_n}) + \sum_{J_\alpha} S_{J_\alpha}^- \\ = (2j+1) (1 + \Delta_+ + \Delta_-) \end{aligned} \quad (57)$$

where the corrections Δ_+ , Δ_- from occupied lower and higher shells, respectively, are

$$\Delta_+ = \frac{1}{A} \sum_{j_1 l_1} S^-(n_1 j_1 l_1 t_3) \begin{pmatrix} j_1 & 1 & j \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}^2$$

$$\left[(2n+2l+1) \delta_{l_1 l-1} \delta_{n_1 n} + 2n \delta_{l_1 l+1} \delta_{n_1 n-1} \right], \quad (58)$$

$$\Delta_- = \frac{1}{A} \sum_{j_1 l_1} S^-(n_1 j_1 l_1 t_3) \begin{pmatrix} j_1 & 1 & j \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}^2$$

$$\left[(2n+2l+3) \delta_{l, l+1} \delta_{n, n} + (2n+2) \delta_{l, l-1} \delta_{n, n+1} \right] \quad (59)$$

When the S^- are taken to be shell model occupation probabilities these results agree to order $1/A$, with corrections obtained directly from Harmonic oscillator shell model wave functions by Bayman and Parish²⁵). This may be taken as confirmation of the fact that our definition of a closed shell, i.e. $\Theta_{nm} = 0$ for all n , agrees with that of the shell model when centre-of-mass corrections are taken into account.

We first evaluate Δ_+ and Δ_- when the relevant major shells,

$n_1 j_1 l_1 t_3$, are completely occupied, i.e. $S^- = 2j_1 + 1$ for all j_1 . The corrections are then independent of $(n j l)$ within a given major shell with total quantum number N given by

$$N = 2n + l .$$

The results are

$$\Delta_+ = N/A , \quad \Delta_- = (N+3)/A \quad (60)$$

If both the adjacent major shells are occupied, as in knockout reactions from deeply bound levels, the net correction is $-3/A$, independent of N . Thus slightly fewer nucleons than $2j_1+1$ can be knocked out of deeply bound levels.

For a valence level where the next shell above is empty, $\Delta_- = 0$, the correction of $+ N/A$ is positive. Although N increases as we move up the periodic table, A increases much faster so that corrections for heavy nuclei are negligible.

Individual contributions to the corrections for the lowest shell model orbitals $(2j_1+1) \Delta_+$, from closed shells $(j_1 l_1)$ are shown in Table 1. To obtain the contribution from a partly closed shell the numbers must be multiplied by $S^-(j_1 l_1)/(2j_1+1)$. The rows add up to $(2j_1+1)N$. From the symmetry of Δ_- and Δ_+ it can easily be verified that the numbers also represent the contributions $(2j_1+1) \Delta_-$ to the sum rules for the $(j_1 l_1)$ -shells from closed shells $(j l)$. Thus the columns sum to $(2j_1+1) (N(j_1 l_1)+3)$.

This symmetry between the contributions of two shells to each others

sum rule also applies if one shell is partly open and has a physical interpretation. We recall that the sum rule (14) states that the sum of spectroscopic factors $\sum_{j\lambda} S^-(j\lambda t_3)$,

is the integral number of appropriate nucleons in the nucleus. Thus, the non-integral $1/A$ corrections must cancel out. As an illustration we give, in Table 2, the number of neutrons in various orbits in ^{16}O and ^{40}Ca , assuming that these are closed shell nuclei. Knockout reactions on these nuclei should theoretically show these minor differences from the shell model values.

We now proceed to examine some experimental data on reactions on light nuclei. Our general conclusion is that uncertainties in reaction analyses preclude at present the unambiguous identification of $1/A$ corrections. Nevertheless their presence does affect the theoretical interpretation of the data.

(a) Knockout reactions on light nuclei.

Nuclei in the $1p$ shell have been the subject of $(p-2p)$ reactions. Two of the most recent analyses of such experiments have been by Tyrén et.al.²⁶⁾ and Jain and Jackson²⁷⁾. Let us assume that these nuclei ranging between ^6Li and ^{16}O have a closed $1s1/2$ shell so that $S^-(1s) = 2$ to zero order. If there are n remaining protons in the p -shell, we use eqs. (57), (58) and (59) to predict that, to order $1/A$, the numbers of p and s shell protons that should be observed experimentally are

$$S^-(1p) = n(1 + 1/A), \quad S^-(1s) = 2 - n/A.$$

The ratios $S^-(1s)/S^-(1p)$ are shown in Table 3. We see that the

ratios differ significantly from the uncorrected ratios. In fact for Li corrections of $O(1/A^2)$ would not be negligible. However, it is unfortunately apparent that present analyses of the data^{26,27)} cannot distinguish between the two values. One might possibly use the improved theoretical value as an aid in making more refined analyses.

(b) Sum rules for closed shell nuclei.

One nucleon transfer reactions on closed shell nuclei such as ^{40}Ca have been used as a test of distorted wave analyses²⁸⁾ and it is very important to know both from the points of view of nuclear structure and of nuclear reactions, how close spectroscopic factors are to their maximum values for these nuclei. The numbers quoted will be $\sum S/(2j+1)$ and are to be compared to unity, the uncorrected shell model value for the sum rule. There is at present controversy between DWBA analyses which give values close to unity and the new Butler theory (BHMM theory) analysis which give considerably smaller values. The smaller values fit in with the views of Brown³⁰⁾ based on a theoretical analysis of Bertsch and Kuo³¹⁾. We give here our views on the subject based on the exact sum rules developed here and in previous papers.

Spectroscopic factors obtained from experiments for ^{16}O $1d_{5/2}$ and ^{40}Ca $1f_{7/2}$ transitions are shown in Table 4 together with the theoretical sums including the $1/A$ corrections obtained from eq. (60). For the latter we have assumed that the $1p_{3/2}$ and $1d_{5/2}$ shells are approximately full in ^{16}O and ^{40}Ca , respectively. We notice that the corrections are positive and not negligible and increase the gaps between theory and experiment. Since our sum rules are exact the gaps

must be filled by the continuum contribution, S_c , if there are no, so far undiscovered, contributions from other bound states. McKellar¹⁷⁾ has estimated continuum contributions to be of the order of 0.1, though his model really needs considerable improvement since it does not take into account energy differences. We hope to examine continuum contributions in detail in a paper in this series but a preliminary estimate¹⁶⁾ agrees with McKellar. The theoretical contributions arising from hard core correlations³⁸⁾ and vibrational coupling³¹⁾ must be contained experimentally in contributions from either other bound states or from the continuum. The experimental absence of any sizeable $f7/2$ strength up to an excitation of 6.8 MeV in ^{41}Ca ³⁹⁾, although three states have been assigned as $f5/2$, argues that contributions from vibrational coupling must be considerably smaller than those estimated by Bertsch and Kuo³¹⁾.

In conclusion we believe that, on present experimental evidence, the values for S^+ based on DWBA theory are much closer to the true values than those obtained from BHMM theory. Indeed it can be argued that the BHMM analysis is inconsistent with McKellar's estimate of the continuum contribution as arising mostly from states with a neutron incident on an excited state of the core¹⁷⁾. The analysis ignores such contributions (M_c' of refs^{3,4)}) relative to the ground state contribution. Furthermore we point out that $1/A$ corrections to the BHMM amplitude, which may not be negligible, can be obtained starting with an exact form for eq. (8) of ref. ⁴⁾ and using a Taylor expansion as in eq. (22) of this paper.

7. Discussion and Conclusions.

The exact relations between overlap functions and spectroscopic factors are given by eqs. (24) and (25) together with the $1/A$ correction given by eqs. (44) and (45). It is first of all remarkable that there should be so many relations between quantities relating adjacent mass nuclei. The uses of these equations have certainly not been exhausted in this paper. The off-diagonal equations are effectively orthogonality relations and we shall show in the next paper of this series how they reduce the problem of representing one-body operators in terms of overlap functions.

We have concentrated here on the diagonal sum rules. The partial sum rules obtained in sect. 4 and whose shell model equivalents were obtained by French⁸⁾ deserve far wider application in nuclear physics than they have had hitherto. They make it really worthwhile for experimentalists to fill in the many gaps in one-nucleon transfer reactions on odd mass nuclei. Indeed we think they are possibly the most powerful theoretical tool for examining valence single particle levels in nuclei together with the consistency and validity of the reaction theories such as DWBA which are used to extract spectroscopic factors from data.

We have shown that the $1/A$ centre-of-mass corrections are significant for the sum rules for light nuclei. They increase the values of spectroscopic factors needed to saturate the sum rules for (valence) single particle levels. In comparison to the original shell model sum rules there are three corrections arising from the exact sum rules. The first is the $1/A$ correction just mentioned. The

second is the occurrence of the factors $|\langle \phi, \phi_n \rangle|^2$ associated with spectroscopic factors. Since the functions are normalized, these factors are strictly less than or equal to unity. This again increases the values of S needed to saturate the sum rules. Just how far the factors differ from unity is a subject for future research which might be tackled by perturbation theory. It would certainly be easy for the DWBA analyst who constructs explicit ϕ_s^2 to examine this point.

In fact we believe the factors will be found to be extremely close to unity except when dealing with levels which are widely split in energy.

Finally there is the unknown contribution of continuum states to the sum rules. The fact that such widely different views on single particle strengths such as ours against Brown's³⁰⁾ and McKellar's¹⁷⁾ (as discussed in sect. 6) can be held at present points out the importance of their further investigation. Whilst we cannot believe at present that such a large fraction as 40% of the strength is in the continuum, we certainly intend to pursue the subject.

Altogether we think that the approach to nuclear physics via overlap functions shows some promise of tying down questions left unanswered by the shell model such as just how big is configurational mixing. The fact that the approach suggests several lines of theoretical work and also new experimental work makes us think it will prove worthwhile.

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Table 1. Sum rule corrections $(2j+1) \Delta_+$ from closed shells $(\lambda_1 j_1)$.

Orbit	Contribution, $A(2j+1) \Delta_+$, from shell $(\lambda_1 j_1)$.					
j	1s1/2	1p3/2	1p1/2	1d5/2	1d3/2	2s1/2
1p3/2	4					
1p1/2	2					
1d5/2		12				
1d3/2		4/3	20/3			
2s1/2		8/3	4/3			
1f7/2				24		
1f5/2				6/5	84/5	
2p3/2				24/5	8/15	20/3
2p1/2					8/3	10/3

Table 2. Numbers of neutrons in closed shells in ^{16}O and ^{40}Ca .

Nucleus	Number in orbit						Total
	1s1/2	1p3/2	1p1/2	1d5/2	1d3/2	2s1/2	
^{16}O	13/8	17/4	17/8				8
^{40}Ca	37/20	37/10	37/20	63/10	21/5	21/10	20

Table 3. Ratio $S^-(1s)/S^-(1p)$ for p-shell nuclei.

Nucleus	n	Ratio	
		Uncorrected = $2/n$	Corrected to $0(1/A)$
${}^6\text{Li}$	1	2	1.57
${}^7\text{Li}$	1	2	1.63
${}^9\text{Be}$	2	1	0.8
${}^{10}\text{B}$	3	0.67	0.52
${}^{11}\text{B}$	3	0.67	0.53
${}^{12}\text{C}$	4	0.5	0.38
${}^{14}\text{N}$	5	0.4	0.31
${}^{16}\text{O}$	6	0.33	0.25

Table 4. Contributions to sum rules $\sum S / (2j+1)$ for light closed shell nuclei.

Target nucleus and orbit	$S^+ / (2j+1)$		$S^- / (2j+1)$	Theoretical sum
	DWBA	BHMM		
^{16}O 1d5/2	0.9 ± 0.1^a	0.45 ± 0.1^b		1.125
^{40}Ca 1f7/2	0.85 ± 0.1^c	0.60 ± 0.1^d	$\leq 0.06^e$	1.075
$a_{\text{refs}}^{32,33)}$	$b_{\text{ref}}^{34)}$	$c_{\text{refs}}^{28,35)}$	$d_{\text{ref}}^{36)}$	$e_{\text{ref}}^{37)}$

Figure Caption.

Fig. 1: Occupancy, n , of an $sl/2$ shell against ratio, r , of sum of spectroscopic factors to states with $J = J_r - 1/2$ to sum for $J = J_r + 1/2$. The excluded regions, in which r_1 and r_2 are the ratios for pickup and stripping reactions, respectively, show that, if n is given, possible values for r_1 and r_2 are restricted.