Group Classification of Many-Body Interactions

C. M. VINCENT*
Department of Applied Mathematics, University of the Witwatersrand, Johannesburg, South Africa
(Received 16 March 1967)

For an n-fermion system in which each particle can occupy any one of k states, an "irreducible b-body operator" is defined as an operator belonging to $[2^b,1^{k-2b}]$ of SU_k. It is shown that such an operator can always be written as a b-body operator multiplied by a function of n. A measure of the failure of a basis to diagonalize the Hamiltonian is constructed. If the Hamiltonian is analyzed into irreducible b-body parts, the measure of error for n particles can be calculated from two-particle parameters. An upper limit on the error of a group theoretically defined basis can be found without having to calculate any n-particle interaction matrix elements. A measure of the magnitude of an interaction is defined, and shown to depend differently on n for irreducible 0-body, 1-body, and 2-body interactions. The effect of the Pauli principle on the formation of shell-model potentials is discussed from this point of view.

1. INTRODUCTION

BOUND-STATE n-body problems in quantum mechanics can be solved approximately by diagonalizing the Hamiltonian in a subspace of Hilbert space constructed as an n-fold product of a single-particle space of finite dimensionality k. The nuclear shell model is an example of this procedure, in which the total capacity of the shells considered is k, and the n-particle states are linear combinations of n-fold products of the k single-particle states. Provided that the system is indeed bound, this approximation can be made arbitrarily good by increasing k sufficiently. We shall assume henceforth that k is large enough for the error due to its finiteness to be negligible.

In practice, the number of n-particle states which must be included is often so large that the Hamiltonian submatrix cannot be diagonalized exactly. Then some approximation must be made. The validity of the approximation is usually checked (if at all) by direct comparison with a more accurate calculation. In this spirit Elliott,[1] for example, checked the accuracy of the SU_3 approximation to the states of F^{19} by comparing them with states obtained by diagonalizing an intermediate coupling Hamiltonian.

This method of estimating the error presupposes the existence of a calculation more accurate than the one being tested. In the important case where the calculation to be tested is already the most accurate one practicable, this method does not apply. There is a need for a method of estimating the error from quantities defined by the calculation itself, without having to make any better calculation.

The main object of this work is to show how to calculate a measure of the error of an approximate diagonalization of a Hamiltonian including two-body interactions. The important quantities turn out to be of the form $\{A|A\}_n \equiv \mathrm{tr}A^\dagger A$, the trace being a sum over all n-particle states. It will be shown that $\{A|A\}_n$ can be expressed in terms of 2-particle quantities, by using the reduction of a 2-body operator into "pure" 0-body, 1-body, and 2-body parts. An essential preliminary is therefore to define the concept of a "pure" b-body operator. This will be done group theoretically by requiring that a "pure" b-body operator belong to a certain irreducible representation (abbreviated IR) of a certain group.

2. CLASSIFICATION OF MANY-BODY FORCES BETWEEN FERMIONS

Let a complete orthonormal set of single-particle states be

$$|1\rangle,\cdots|m\rangle,\cdots|k\rangle. \tag{1}$$

We denote the k-dimensional space spanned by these states by L_k. Although k must be finite, it can be as large as necessary to make the approximation good.

We consider the case of identical fermions. Then for each basic state $|m\rangle$, an operator $f_m^\dagger$ can be defined which creates a fermion in that state. These operators satisfy the anticommutation rules

$$\begin{aligned}&[f_m^\dagger,f_{m'}^\dagger]_+=[f_m,f_{m'}]_+=0,\\ &[f_m,f_{m'}^\dagger]_+=\delta_{mm'}.\end{aligned} \tag{2}$$

A state of n-particles can be expressed in the form of a homogeneous polynomial of degree n acting on the vacuum state $|0\rangle$:

$$n\text{-particle state}=P_n(f_1^\dagger\cdots f_k^\dagger)|0\rangle. \tag{3}$$

Consider a transformation on L_k defined by its effect on the $|m\rangle$:

$$U|m\rangle=\sum_{m'} U_{m'm}|m'\rangle.$$

If $U_{m'm}$ is a unitary matrix, the $U|m\rangle$ are a new orthonormal basis. The set of all such transformations is U_k, the unitary group in k dimensions. If we restrict ourselves to transformations for which $U_{m'm}$ has unit determinant, the group is SU_k.

The creation operators transform as a vector under SU_k, that is, they belong to the irreducible representa-

* Present address: Department of Physics, The Weizmann Institute of Science, Rehovoth, Israel.

[1] J. P. Elliott, Proc. Roy. Soc. (London) **A245**, 128 (1958).

tion (IR) labeled by the Young partition $[1]$:

$$U f_m^\dagger U^{-1}=\sum_{m'} U_{m'm} f_{m'}^\dagger, \tag{4}$$

and

$$f_m^\dagger \sim [1], \tag{5}$$

where the symbol $\sim$ means "belongs to." Therefore, a product of n of the anticommuting $f_m^\dagger$ belongs to the IR of antisymmetric tensors of order n, namely $[1^n]$. So by (3) an n-particle state belongs to $[1^n]$. This condition is just an expression of the Pauli principle.

A general b-body operator is one expressible as a sum of terms, each of which depends on the coordinates of a different set of b particles; thus,

$$A^{(n)}=\sum_{n\geqslant i_1>i_2>\cdots>i_b\geqslant 1} A(i_1\cdots i_b), \tag{6}$$

Every operator symmetric in all particles can be expanded in terms of creation and annihilation operators $f_m^\dagger$ and f_m. The second-quantization form of a general b-body operator is

$$A=\sum f_{m_1}^\dagger\cdots f_{m_b}^\dagger A_{m_1\cdots m_b}^{m_1'\cdots m_b'} f_{m_1'}\cdots f_{m_b'}, \tag{7}$$

where the sum is over all repeated indices.

Consider the SU_k transformation properties of (7). The product of b anticommuting creation operators is a component of an antisymmetric tensor of order b, and therefore belongs to $[1^b]$ of SU_k. The product of b anticommuting annihilation operators belongs to the complex conjugate representation $[1^b]^*$ which is equivalent to $[1^{k-b}]$. Therefore,

$$\begin{aligned} A&\sim[1^b]\times[1^{k-b}]\\ &=I+[2,1^{k-2}]+[2^2,1^{k-4}]+\cdots\\ &\qquad+[2^{k-b},1^{2b-k}]\,(b>k/2), \qquad (8a)\\ &=I+[2,1^{k-2}]+[2^2,1^{k-4}]+\cdots\\ &\qquad+[2^b,1^{k-2b}]\,(b\leqslant k/2), \qquad (8b)\end{aligned}$$

where I is the identity representation. The Kronecker product has been reduced by the rules given for example by Hamermesh.[2] Since only small values of b are of interest, we may suppose that k is large enough for (8b) to apply. Then the complexity of IR's appearing is limited by b and not by k.

An irreducible b-body operator is now defined as any operator belonging to an IR of SU_k contained in the reduction of the representation to which a general b-body operator belongs, but not contained in the reduction of the representation to which a general $(b-1)$-body operator belongs.

Replacing b by $b-1$ in (8b), it follows that

$$\textit{irreducible b-body operator}\sim[2^b,1^{k-2b}] \text{ of } SU_k. \tag{9}$$

Can every operator belonging to $[2^b,1^{k-2b}]$ be written in the form of a b-body operator? If not, the definition (9) is inappropriate because then an "irreducible b-body operator" need not necessarily be a b-body operator at all. The answer is contained in the following theorem:

Theorem 1: If A is an operator belonging to $[2^b,1^{k-2b}]$ of SU_k, then it can be written in b-body form (i.e., as a b-body operator times a function of n).

Proof: Denote $[2^b,1^{k-2b}]$ by D^b for short.

Let A be a member of a space L^b of operators, providing an IR D^b of SU_k.

Since D^b is one of the IR's contained in the reduction of the representation to which a general b-body operator belongs, there will exist some b-body operator belonging to D^b, say,

$$B\sim D^b.$$

Let B belong to a space M^b of operators, providing an IR D^b of SU_k. Since D^b is irreducible, any vector of M^b can be expanded in terms of the vectors obtained by letting the elements U of SU_k act on B.

There will be a vector $\bar{A}$ in M^b belonging to the same row of D^b as A in L^b, and $\bar{A}$ can be expanded in the form

$$A=\int dU\; C(U)UBU^{-1}=\int dU\; C(U)UBU^\dagger,$$

where $C(U)$ is a number depending on the element U.

B is b-body, and U induces a linear transformation on the $f_m^\dagger$ and f_m by (4). Therefore $UBU^\dagger$ is also an expression of degree b in the $f_m^\dagger$ and in the f_m, that is, by (7), a b-body operator. Therefore $\bar{A}$ is a b-body operator.

Now A and $\bar{A}$ are both operators on the same irreducible representation space for SU_k, namely the space of antisymmetric tensors of order n, belonging to $[1^n]$. A and $\bar{A}$ belong to the same row of the same IR D^b of SU_k. The Kronecker product $D^b\times[1^n]$ is simply reducible, that is, it contains no IR more than once. In this situation, the Wigner-Eckart[3] theorem applies. It states that A and $\bar{A}$ are equal up to a scalar numerical factor;

$$A=a\bar{A}.$$

The factor a may depend on n.

Since $\bar{A}$ is b-body, this expresses A in b-body form, and theorem 1 is proved.

It is worth noticing that the simple reducibility of $D^b\times[1^n]$ is essential to the argument. For this reason the theory cannot be worked out without taking quantum-mechanical symmetrization into account. Theorem 1 would go through for bosons, because $D^b\times[n]$ is also simply reducible.

As a simple illustration of theorem 1, consider a 1-body operator belonging to the 0-body IR I of SU_k. By (7), it is a bilinear expression in the $f_m^\dagger$ and f_m, belonging to I. Since $f_m\sim[1]$ and $f_m^\dagger\sim[1]^*$, and the product

[2] M. Hamermesh, *Group Theory* (Pergamon Press, Ltd., London, 1962).

[3] E. P. Wigner, Z. Physik **43**, 624 (1927); C. Eckart, Rev. Mod. Phys. **2**, 305 (1930).

$[1]\times[1]^*$ contains I once only, there is one and only one way to construct such a bilinear expression belonging to I, namely

$$\sum f_m^\dagger f_m = n = \text{number of particles}.$$

But since this depends only on the number of particles, and not at all on the states they occupy, it has been written in 0-body form, in accordance with theorem 1. This also illustrates our convention that if A is a b-body operator, then $a(n)A$ is considered to be in b-body form, for any function a of the number of particles.

3. TRACES OF IRREDUCIBLE b-BODY OPERATORS

In the evaluation of the trace of the square of an operator for n particles, quantities like $\sum A_{pm}{}^{qm}$ occur, where A is an irreducible 2-body operator and m is summed over all single-particle states. If one sets any upper index equal to any lower index of a b-body operator, and sums, the result is called a trace of the operator. Then the following applies:

Theorem 2: Every trace of an *irreducible* b-body operator vanishes for $b \geqslant 1$.

Proof: To avoid notational difficulties, we consider the case of an irreducible 2-body operator, with matrix $A_{pr}{}^{qs}$, supposing that one of its traces, say

$$\sum A_{pm}{}^{qm} \equiv B_p{}^q \neq 0.$$

From this trace one can then construct a 1-body operator,

$$B = \sum f_p^\dagger B_p{}^q f_q.$$

Since the matrix elements defining B are obtained by taking linear combinations of the matrix elements defining A, B belongs to a representation contained in the representation to which A belongs. Since A is irreducible 2-body,

$$A \sim [2^2, 1^{k-4}].$$

Therefore,

$$B \sim [2^2, 1^{k-4}].$$

But no 1-body operator can belong to this IR. The contradiction shows that $B \neq 0$ is false. Therefore,

$$\sum A_{pm}{}^{qm} = 0.$$

The extension to arbitrary b is straightforward. If some trace of an irreducible b-body operator does not vanish, one can construct a $(b-1)$-body operator belonging to a representation contained in $[2^b, 1^{k-2b}]$ and therefore equivalent to it. But no $(b-1)$-body operator can belong to this IR. The vanishing of the trace follows. Conversely, every b-body operator with all traces vanishing is an irreducible b-body operator.

4. ESTIMATING THE ACCURACY OF A DIAGONALIZATION

Let H be the n-particle Hamiltonian, and consider the complete orthonormal set of p n-particle states $|i\rangle$ as approximations to the eigenstates of H. Let (H_{ij}) be the representative matrix of H in this basis, so that

$$H|i\rangle = \sum_j H_{ji}|j\rangle. \tag{10}$$

Denote the eigenvector of H nearest to $|i\rangle$ by $|\bar{\imath}\rangle$, so that

$$H|\bar{\imath}\rangle = E_i|\bar{\imath}\rangle. \tag{11}$$

First-order perturbation theory is valid for the calculation of $|\bar{\imath}\rangle - |i\rangle$ provided that this difference is small. It gives

$$|ei\rangle \equiv |\bar{\imath}\rangle - |i\rangle = \sum_{j\neq i} H_{ji}|j\rangle/(E_i - E_j).$$

The replacement of the energy denominator $H_{ii}-H_{jj}$ by E_i-E_j introduces no first-order error. The average square of the error vector is

$$e^2 \equiv p^{-1}\sum\langle ei|ei\rangle = p^{-1}\sum_{i\neq j}|H_{ij}|^2/(E_i-E_j)^2. \tag{12}$$

The summation is now over both i and j.

We replace $(E_i-E_j)^2$ by its average value

$$\langle (E_i-E_j)^2\rangle = p^{-2}\sum_{ij}(E_i^2+E_j^2-2E_iE_j).$$

This expression is invariant under the addition of a constant to H, so we may replace H by its traceless part H_{1+2}. Then

$$\langle (E_i-E_j)^2\rangle = 2p^{-1}\,\mathrm{tr}H_{1+2}{}^2,$$

which gives in (12)

$$e^2 = \tfrac{1}{2}\sum_{i\neq j}|H_{ij}|^2/\mathrm{tr}H_{1+2}{}^2. \tag{13}$$

It is interesting to see that if we define an error vector

$$|\chi i\rangle = H|i\rangle - H_{ii}|i\rangle$$

then a new measure of the total error results, namely

$$x^2 \equiv \sum\langle\chi i|\chi i\rangle = \sum\langle i|H^2|i\rangle - \sum H_{ii}{}^2 = \sum_{i\neq j}|H_{ij}|^2,$$

the numerator of (13).

Equation (13) was derived using perturbation theory, and is invalid if the states $|i\rangle$ are very different from the states $|\bar{\imath}\rangle$. It also suffers from the replacement of $(E_i-E_j)^2$ by its average value in the denominator. These difficulties could be avoided by the use of x^2 as a measure of error. However, x^2 cannot be simply interpreted in terms of mixture of basis states.

Since the trace of the square of H plays such an important part in the theory, we define

$$\{A|B\} = \mathrm{tr}A^\dagger B. \tag{14}$$

This satisfies the requirements for a scalar product. In this sense we can refer to $\{A|A\}$ as the "norm" of the operator A, and regard it as a measure of the magnitude

of A. A similar measure has been used by Hoffmann[4] in a general discussion of approximations in quantum mechanics.

In the new notation, (13) becomes

$$e^2=\tfrac{1}{2}[\{H|H\}-\sum H_{ii}{}^2]/\{H_{1+2}|H_{1+2}\}. \quad (15)$$

This result shows that given a basis $|i\rangle$, one can estimate how accurately it diagonalizes H by calculating $\{H|H\}$, $\sum H_{ii}{}^2$, and $\{H_{1+2}|H_{1+2}\}$. It will be shown that it is possible to calculate $\{H|H\}$ and $\{H_{1+2}|H_{1+2}\}$ quite simply for n particles from parameters of H which can be evaluated in the 2-particle case. Then it is only necessary to calculate $\sum H_{ii}{}^2$, which involves only the diagonal elements. Thus it will be possible to estimate the error of a diagonalization *without knowing any of the n-particle off-diagonal matrix elements*. The fact that all the diagonal elements must be calculated is a drawback, but even this difficulty can be removed if one is satisfied with an approximate upper limit on e^2.

A common and convenient way of defining an orthonormal basis is to find a group G (a subgroup of SU_k) under which H is almost invariant. Elliott's SU_3 is a well-known example of this.[1] Then H can be analyzed into a part belonging to a sum of nonidentity IR's of G; and an invariant part.

$$H=H_I+H', \quad (16a)$$

where

$$H_I\sim I,\ H'\sim\text{sum of IR's}\neq I. \quad (16b)$$

Then the basis $|i\rangle$ can be chosen to diagonalize H_I:

$$\langle i|H_I|j\rangle=0 \quad \text{for} \quad i\neq j. \quad (17)$$

From (16) and (17)

$$\sum_{i\neq j}|H_{ij}|^2=\sum_{i\neq j}|\langle i|H'|j\rangle|^2\leqslant\sum_{ij}|\langle i|H'|j\rangle|^2=\{H'|H'\}.$$

Substituting this in (13), an upper limit on e^2 [as given by (13)] results:

$$e^2\leqslant\tfrac{1}{2}\{H'|H'\}/\{H_{1+2}|H_{1+2}\}. \quad (18)$$

The problem of estimating the error of the diagonalization is now reduced to the calculation of the n-particle norms of the traceless part of H and its G-noninvariant part. It is not necessary to calculate *any* n-particle matrix elements, diagonal or otherwise.

One caution should be applied to the use of this method. This is that e^2 is only an average estimate of the error in any given approximate eigenvector. The actual error in a particular case may be much higher than its average value, although we may hope "on statistical grounds" that this is unlikely.

[4] T. A. Hoffmann, Phil. Trans. Roy. Soc. London **257A**, 309 (1965).

5. NORMS OF 2-BODY OPERATORS FOR n-PARTICLE SYSTEMS

If A and B are operators on n-particle states, we denote their scalar product by $\{A|B\}_n$. Neglecting the possibility of 3-body interactions, the operators we deal with are at most 2-body, and as such can be analyzed into irreducible 0-body ,1-body, and 2-body parts. This process corresponds to the ordinary reduction of a representation space for $I+[2,1^{k-2}]+[2^2,1^{k-4}]$ of SU_k to its irreducible subspaces. Thus

$$A=A_0+A_1+A_2, \quad (19)$$

and similarly for B.

We note the selection rule on $\{A|B\}$, if A and B both belong to IR's of SU_k or any subgroup:

$$A\sim D^\alpha, \quad B\sim D^\beta. \quad (20)$$

Since by (14) $\{A|B\}$ is constructed as a trace,

$$\{A|B\}\sim I.$$

But by (14) and (20),

$$\{A|B\}\sim D^{\alpha*}\times D^\beta.$$

Therefore $\{A|B\}$ vanishes unless $D^{\alpha*}\times D^\beta$ contains I, that is

$$\{A|B\}=0 \quad \text{unless} \quad D^\alpha\equiv D^\beta. \quad (21)$$

Using the distributivity of the scalar product and (21), we get

$$\{A|B\}_n=\{A_0|B_0\}_n+\{A_1|B_1\}_n+\{A_2|B_2\}_n, \quad (22)$$

so that the parts of different b contribute independently to the scalar product. We can therefore treat the parts of different b separately.

Suppose that A_b and B_b ($b=0$, 1, 2) are irreducible b-body operators, given by

$$A_0=A, \quad (23a)$$

$$A_1=\sum f_p{}^\dagger A_p{}^q f_q, \quad (23b)$$

$$A_2=\sum f_p{}^\dagger f_q{}^\dagger A_{pq}{}^{rs} f_r f_s, \quad (23c)$$

with similar equations for the B_b. Then we shall show that

$$\{A_0|B_0\}_n={}^kC_n A^*B, \quad (24a)$$

$$\{A_1|B_1\}_n={}^{k-2}C_{n-1}\sum A_p{}^q{}^*B_p{}^q, \quad (24b)$$

$$\{A_2|B_2\}_n={}^{k-4}C_{n-2}\sum A_{pq}{}^{rs}{}^*B_{pq}{}^{rs}\times 4, \quad (24c)$$

with

$${}^kC_n=k!/[n!(k-n)!]. \quad (25)$$

The proof of (24a) is trivial, depending only on the fact that there are ${}^kC_n$ independent n-particle states.

To prove (24b), we remark first that since A_1 and B_1 are irreducible 1-body operators, their traces vanish by theorem 2. Therefore $\sum A_p{}^q{}^*B_p{}^q$ is the only bilinear SU_k invariant which can be constructed from them. So the bilinear invariant $\{A_1|B_1\}_n$ is proportional to this

quantity. The factor of proportionality must depend only on k and n, and not at all on the detailed forms of A_1 and B_1. To calculate this factor of proportionality we can replace A_1 and B_1 by any convenient irreducible 1-body operator. We take

$$A_1=B_1=f_1^\dagger f_2, \tag{26a}$$

for which

$$\sum A_p{}^q{}^* B_p{}^q=1. \tag{26b}$$

Then using (14) and (2),

$$\{A_1|B_1\}_n=\mathrm{tr}(f_2^\dagger f_1 f_1^\dagger f_2)=\mathrm{tr}[(1-n_1)n_2],$$

where

$$n_m=f_m^\dagger f_m$$

is the occupation number of state $|m\rangle$, and has eigenvalues 0 and 1. We evaluate the trace in the n-particle basis

$$|m_1\cdots m_n\rangle=f_{m_1}^\dagger\cdots f_{m_n}^\dagger|0\rangle, \tag{27}$$

$$\{A_1|B_1\}_n=\sum_{m_1\cdots m_n}\langle m_1\cdots m_n|(1-n_1)n_2|m_1\cdots m_n\rangle.$$

The matrix element is 1 if $n_2=1$ and $n_1=0$, and zero otherwise. The number of surviving terms is the number of ways of selecting n numbers $m_1\cdots m_n$ from 1, 2, $\cdots k$, under the condition that one of them is 2 and none of them is 1. Since 2 is certainly selected, only $n-1$ numbers remain to be chosen. Since none of these $n-1$ may be either 1 or 2, they must be selected from 3, 4, $\cdots k$, which can be done in ${}^{k-2}C_{n-1}$ ways. Therefore

$$\{A_1|B_1\}_n={}^{k-2}C_{n-1}={}^{k-2}C_{n-1}\sum A_p{}^q{}^* B_p{}^q$$

by (26b), proving (24b).

In the same way $\sum A_{pq}{}^{rs}{}^* B_{pq}{}^{rs}$ is the only bilinear SU_k invariant which can be constructed from the irreducible 2-body operators A_2 and B_2, where $A_{pq}{}^{rs}$ and $B_{pq}{}^{rs}$ are antisymmetric in upper and lower indices separately. Replacing A_2 and B_2 by any simple irreducible 2-body operators, we can again calculate the universal proportionality factor between $\{A_2|B_2\}_n$ and $\sum A_{pq}{}^{rs}{}^* B_{pq}{}^{rs}$. We take

$$A_2=B_2=f_1^\dagger f_2^\dagger f_3 f_4=\tfrac{1}{4}(f_1^\dagger f_2^\dagger f_3 f_4-f_2^\dagger f_1^\dagger f_3 f_4 + f_2^\dagger f_1^\dagger f_4 f_3-f_1^\dagger f_2^\dagger f_4 f_3), \tag{28a}$$

for which

$$\sum A_{pq}{}^{rs}{}^* B_{pq}{}^{rs}=\tfrac{1}{4}. \tag{28b}$$

Then

$$\{A_2|B_2\}_n=\mathrm{tr}(f_4^\dagger f_3^\dagger f_2 f_1 f_1^\dagger f_2^\dagger f_3 f_4),$$
$$=\mathrm{tr}[(1-n_1)(1-n_2)n_3 n_4],$$
$$=\sum\langle m_1\cdots m_n|(1-n_1)(1-n_2)n_3 n_4|m_1\cdots m_n\rangle.$$

The matrix element is 1 if $n_1=n_2=0$ and $n_3=n_4=1$, and zero otherwise. In the same way as before, the number of surviving terms is the number of ways of choosing $n-2$ numbers from 5, 6, $\cdots k$, that is ${}^{k-4}C_{n-2}$. Therefore using (28b),

$$\{A_2|B_2\}_n={}^{k-4}C_{n-2}={}^{k-4}C_{n-2}4\sum A_{pq}{}^{rs}{}^* B_{pq}{}^{rs},$$

which is (24c). The general result for arbitrary b is

$$\{A_b|B_b\}_n=(b!)^2\times{}^{k-2b}C_{n-b}\times\sum(A_{pq\ldots}{}^{rs\cdots})^*(B_{pq\ldots}{}^{rs\cdots}). \tag{29}$$

We now show how the Eq. (24) permits the calculation of the quantities $\{H|H\}$, $\{H'|H'\}$, and $\{H_{1+2}|H_{1+2}\}$, which occur in (15) and (18). The Hamiltonian is assumed to be the sum of a general 1-body and a general 2-body operator:

$$H=H^{(1)}+H^{(2)}. \tag{30}$$

Its irreducible 0-body, 1-body, and 2-body parts are

$$\begin{aligned} H_0&=H_0{}^{(1)}+H_0{}^{(2)},\\ H_1&=H_1{}^{(1)}+H_1{}^{(2)},\\ H_2&=H_2{}^{(2)}, \end{aligned} \tag{31}$$

where $H_b{}^{(a)}$ is the irreducible b-body part of the general a-body operator $H^{(a)}$. We consider irreducible 0-body, 1-body and 2-body parts in turn.

Irreducible 0-Body

$$\begin{aligned} H_0{}^{(1)}&=nh(1),\\ H_0{}^{(2)}&=\tfrac{1}{2}n(n-1)h(2), \end{aligned} \tag{32}$$

where $h(1)$ and $h(2)$ are constants (independent of n) since n and $\frac{1}{2}n(n-1)$ are, respectively, the numbers of terms in the expansion (6) of general 1-body and 2-body operators.

By (24a)

$$\{H_0|H_0\}_n={}^kC_n|nh(1)+\tfrac{1}{2}n(n-1)h(2)|^2$$
$$={}^kC_n[n^2|h(1)|^2+\mathrm{Re}n^2(n-1)h(1)^*h(2)+\tfrac{1}{4}n^2(n-1)^2|h(2)|^2]. \tag{33}$$

Applying (24a) to (32) for $n=2$,

$$\begin{aligned} \{H_0{}^{(1)}|H_0{}^{(1)}\}_2&=2k(k-1)|h(1)|^2,\\ \{H_0{}^{(1)}|H_0{}^{(2)}\}_2&=k(k-1)h(1)^*h(2),\\ \{H_0{}^{(2)}|H_0{}^{(2)}\}_2&=\tfrac{1}{2}k(k-1)|h(2)|^2. \end{aligned} \tag{34}$$

Substituting these in (33),

$$\{H_0|H_0\}_n={}^kC_n[n^2\{H_0{}^{(1)}|H_0{}^{(1)}\}_2+\mathrm{Re}2n^2(n-1)\{H_0{}^{(1)}|H_0{}^{(2)}\}_2+n^2(n-1)^2\{H_0{}^{(2)}|H_0{}^{(2)}\}_2]/[2k(k-1)]. \tag{35}$$

Irreducible 1-Body

$$H_1{}^{(1)}=\sum f_p^\dagger h(1)_p{}^q f_q, \tag{36a}$$

$$H_1{}^{(2)}=\sum_{n\geq i>j\geq 1}[H(i)+H(j)]=(n-1)\sum_{i=1}^{n}H(i)$$
$$=(n-1)\sum f_p^\dagger h(2)_p{}^q f_q. \tag{36b}$$

Here use has been made of the fact that $H_1^{(2)}$ can be written in 1-body form. The h's are again independent of n. By (24b) and (36),

$$\{H_1|H_1\}_n = {}^{k-2}C_{n-1}\sum|h(1)_p{}^q+(n-1)h(2)_p{}^q|^2$$
$$= {}^{k-2}C_{n-1}[\sum|h(1)_p{}^q|^2+2(n-1)$$
$$\times\mathrm{Re}\sum h(1)_p{}^{q*}h(2)_p{}^q+(n-1)^2\sum|h(2)_p{}^q|^2].$$

Applying (24b) to 36a) and (36b) for $n=2$,

$$\{H_1^{(1)}|H_1^{(1)}\}_2=(k-2)\sum|h(1)_p{}^q|^2,$$
$$\{H_1^{(1)}|H_1^{(2)}\}_2=(k-2)\sum h(1)_p{}^{q*}h(2)_p{}^q, \quad (37)$$
$$\{H_1^{(2)}|H_1^{(2)}\}_2=(k-2)\sum|h(2)_p{}^q|^2.$$

Substituting (37) in the expression for $\{H_1|H_1\}_n$,

$$\{H_1|H_1\}_n = {}^{k-2}C_{n-1}(k-2)^{-1}[\{H_1^{(1)}|H_1^{(1)}\}_2$$
$$+2(n-1)\,\mathrm{Re}\{H_1^{(1)}|H_1^{(2)}\}_2$$
$$+(n-1)^2\{H_1^{(2)}|H_1^{(2)}\}_2]. \quad (38)$$

Irreducible 2-Body

Putting $H_2^{(2)}$ for A_2 and B_2 in (24c) and comparing with the result for $n=2$,

$$\{H_2|H_2\}_n=\{H_2^{(2)}|H_2^{(2)}\}_n \quad (39)$$
$$= {}^{k-4}C_{n-2}\{H_2^{(2)}|H_2^{(2)}\}_2.$$

Considering now the quantities $\{H|H\}_n$, $\{H'|H'\}_n$, and $\{H_{12}|H_{12}\}_n$ occurring in the formulas for the measure of error e^2, we have first

$$\{H|H\}_n=\{H_0|H_0\}_n+\{H_1|H_1\}_n+\{H_2|H_2\}_n, \quad (40)$$

where the quantities on the right-hand side are given by (35), (38), and (39). The traceless part of

$$H=H_0+H_1+H_2$$

is

$$H_{1+2}=H_1+H_2, \quad (41)$$

since H_0 is a scalar and H_1 and H_2 are traceless by (21). So

$$\{H_{12}|H_{12}\}_n=\{H_1|H_1\}_n+\{H_2|H_2\}_n \quad (42)$$

and the right-hand side is evaluated by (38) and (39). Lastly, H' is the part of H which belongs to a sum of IR's of a subgroup G of SU_k other than I. Let

$$H'=H_1'+H_2',$$

where H_b' is the pure b-body part of H'. H_0' is necessarily zero, because H' is traceless by (21), since it belongs to IR's of G other than I. Then

$$\{H'|H'\}_n=\{H_1'|H_1'\}_n+\{H_2'|H_2'\}_n \quad (43)$$

and the separate parts can again be determined from (38) and (39).

The prescription for calculating the measure of error e^2 for n-particle systems in terms of 2-particle quantities is now complete. The reduction of the 2-particle operators to irreducible b-body parts is the only step which may involve appreciable computation.

Suppose the matrix $A_{pq}{}^{rs}$ of a general 2-body operator has been constructed explicitly. Then the matrices of 1-body and 0-body operators can be constructed:

$$A(1)_{pq}{}^{rs}=\sum_m[A_{mq}{}^{ms}\delta_{pr}+A_{mq}{}^{rm}\delta_{ps}$$
$$+A_{pm}{}^{ms}\delta_{qr}+A_{pm}{}^{rm}\delta_{qs}],$$
$$A(0)_{pq}{}^{rs}=\sum_{lm}A_{lm}{}^{lm}[\delta_{pr}\delta_{qs}-\delta_{ps}\delta_{qr}].$$

Like $A_{pq}{}^{rs}$, these are antisymmetric in pq and rs. The irreducible 2-body part of A then has the matrix

$$A(2)_{pq}{}^{rs}=A_{pq}{}^{rs}-A(1)_{pq}{}^{rs}/(k-2)$$
$$+A(0)_{pq}{}^{rs}/[(k-1)(k-2)].$$

The fact that this is irreducible 2-body follows from the vanishing of its traces, which can be verified.

The irreducible 1-body and 0-body parts of A can be found in the same way.

In cases where the interaction has been analyzed into parts belonging to IR's of a subgroup of SU_k, this analysis can often be used to facilitate the SU_k analysis.

6. NORM OF A GENERAL 2-BODY INTERACTION

Consider a general 2-body interaction:

$$V=\sum_{n\geq i>j\geq 1}V(ij)=V_0+V_1+V_2, \quad (44)$$

where V_b is the irreducible b-body part of the interaction. $\{V|V\}_n$ can be calculated by the techniques of the last section. One puts $H_b{}^{(1)}=0$ and $H_b{}^{(2)}=V_b$ for $b=0$, 1, 2 in (35), (38), and (39). Applying (22) to the result gives

$$\{V|V\}_n=\frac{(k-4)!}{(k-n-2)!(n-2)!}$$
$$\times\left[\frac{(k-2)(k-3)}{(k-n)(k-n-1)}\frac{n(n-1)}{2}\{V_0|V_0\}_2\right.$$
$$\left.+\frac{k-3}{k-n-1}(n-1)\{V_1|V_1\}_2+\{V_2|V_2\}_2\right]. \quad (45)$$

French[5] has given a result resembling (45). In our notation it essentially expresses $\{V|V\}_n$ in terms of $\{V|V\}_{k-1}$, $\{V|V\}_1$, and $\{V|V\}_2$. For pure 0-body, 1-body, and 2-body interactions French's result is consistent with (45). Special cases of French's result have been given by Moszkowski[6] and Layzer.[7]

The result (45) can be used to suggest a reason for the validity of shell models for bound states of many-fermion systems. Consider a system of n fermions in-

[5] J. B. French, Phys. Letters **23**, 248 (1966).
[6] S. A. Moszkowski, Progr. Theoret. Phys. (Kyoto) **28**, 1 (1962).
[7] D. Layzer, Phys. Rev. **132**, 2125 (1963).

teracting through the 2-body potential V, so that

$$H=\sum_{i=1}^{n} T(i)+\sum_{n\geq i>j\geq 1} V(ij), \tag{46}$$

where $T(i)$ is the kinetic energy of the ith particle. For the lowest bound states of the system we assume that:

(a) The system can be placed at the center of an impenetrable sphere of large radius, without appreciably changing its properties. Then the eigenstates of a free particle in the sphere can be used as a single-particle basis.

(b) The probability of occupation of single-particle states above a certain kinetic energy is negligible. Then the infinite discrete set of sphere eigenstates can be replaced by a finite set of k states.

The theory leading to (45) now applies. Assume that V has a nonvanishing irreducible 1-body part. Because of the different n dependence of the factors in (45), when n is large the 1-body and 0-body parts of V soon swamp the irreducible 2-body part, and dominate V.

For n large enough, the interaction will be effectively a mixture of irreducible 0-body and 1-body parts. By theorem 1 it can be written in the form

$$V=\sum_{i} V(i), \tag{47}$$

so that

$$H=\sum_{i=1}^{n} [T(i)+V(i)]. \tag{48}$$

The eigenstates of this independent-particle Hamiltonian will simply be Slater determinants.

This discussion suggests that independent particle motion should always be a good approximation for large enough n, provided only that the irreducible 1-body part of the interaction does not vanish. But the situation is not really so simple. For example, (45) predicts that $V(i)$ varies in strength with n, but its form must be independent of n, as can be seen from (36b). But in the nuclear shell model, for instance, the potential has to be almost constant in depth, but increasing in range as $n^{1/3}$. This paradox arises because $\{V\,|\,V\}_n$ is an *average* measure of the magnitude of the interaction, averaged over *all* states of the system. Now k is much greater than n for some relevant values of n. Then most of the states do not resemble the nuclear ground state at all, but are more like states of many particles moving almost freely inside the sphere. So the $V(i)$ of (48) cannot be expected to resemble the shell-model potential for the ground state.

The derivation of (48) uses the Pauli principle at two critical points. Theorem 1 cannot be proved without quantum statistics, and the relations (24) would be quite different for bosons. The Brueckner[8] approach to the justification of the shell model also relies on the Pauli principle to prohibit many scattering processes. It would be interesting to derive (24) for bosons, and see if the argument leading to (48) breaks down for this case.

In discussing general questions the need to truncate the single-particle configuration space is irksome. Possibly a mathematical method can be developed for extending the definition of irreducible b-body operators to the infinite-dimensional configuration space. Then the reduction of an operator will not depend on the way the configuration space is truncated.

ACKNOWLEDGMENTS

This work was done during the tenure of an Ernest Oppenheimer Memorial Fellowship, for which I am very grateful to the Ernest Oppenheimer Memorial Trust, Johannesburg.

[8] K. A. Brueckner and C. A. Levinson, Phys. Rev. **97**, 1344 (1955); K. A. Brueckner, *ibid.* **97**, 1353 (1955); **100**, 36 (1955).