Automated algebra for higher order perturbation diagrams with angular momentum coupling

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The use of Wick's theorem and angular momentum recoupling rules to construct perturbative algebraic expressions for the shell-model effective interaction is discussed. The problem is shown to reduce to the evaluation of certain configuration traces, which can be accomplished by techniques previously developed for use in trace-moment statistical spectroscopy. The use of the existing configuration-trace symbol-manipulation programs for automatic generation of complete sets of optimally simplified expressions is summarized. Examples are presented of expressions for fourth-order diagrams and of the simplifications achieved for third-order diagrams.

I. INTRODUCTION

Perturbation theory has been the basis of almost all effective interaction and effective operator calculations. However, the complexities of the higher order terms are such that complete calculations have only been done up to the third order. Until now, even the algebraic expressions for all the fourth order terms have not been worked out. The main difficulty seems to be the sheer volume and intricacy of the manipulations involved. Typically one starts with the m scheme because of the ease of carrying out the commutations and contractions of the single particle creation and annihilation operators. On the other hand, the final expressions for the matrix elements must be in the angular momentum coupled representation so as to exploit angular momentum conservation. This can be done by the use of Clebsch-Gordan coefficients, and for the low order terms this is indeed a good way to proceed. However, the method is impractical for the higher order terms, which are needed for control of truncation errors.[1]

Recently Kuo *et al.*[2] devised a method to evaluate perturbation diagrams in the coupled representation using ingenious techniques to decompose a diagram into ladder diagrams and then express each ladder diagram in the coupled representation. Although it is a major improvement over the m-scheme approach, it still involves a painstaking search for all the basic diagrams, then the decomposition of each diagram, and finally angular momentum recouplings. Furthermore, there is usually more than one way to carry out the algebra and, in general, different approaches can produce different forms of the final results. Needless to say, it is very important to find the simplest final expression, both for aesthetic reasons and for economy of numerical computational time.

In this paper we show that the problem can be reduced to one which has already been completely solved in the context of statistical spectroscopic theory. The desired matrix element is in fact a special case of a configuration trace. The method developed for this problem makes use of a computer to carry out the tedious work of finding all the basic diagrams and performing all the contractions and associated angular momentum recouplings. Since the work is done by a machine, we are afforded the luxury of exploring all possibilities so as to arrive at the simplest final forms. As a result, many terms acquire simpler forms by the use of our approach, compared with the results given by Barrett and Kirson.[3]

The method consists of two parts. Firstly, for a particular perturbation order, we find by symmetry considerations all the basic or topologically distinct diagrams. Secondly, for each diagram, the algebraic expression is derived completely in the coupled scheme; no magnetic projection quantum number m appears anywhere and no Clebsch-Gordan coefficient is used in any way. All recouplings are carried out in terms of 6-J symbols and, in order to make use of further sum rules, 9-J symbols. The program has built into it the ability to recognize algebraically all the angular momentum recoupling sum rules up to and including 9-J symbols.

As mentioned, the computer programs were originally written for obtaining configuration trace expressions for a product of excitation operators and Hamiltonians.[4,5] We need only apply the close connection between trace and perturbation diagrams (given in Sec. II) to produce the effective-interaction results. Since the methods for configuration traces are fully reported in Ref. 4, we shall here be content to summarize them (see Sec. III). Expressions for the third order effective interaction terms and some selected examples of fourth order terms are discussed in Sec. IV. A brief concluding discussion is given in Sec. V.

II. EFFECTIVE INTERACTIONS AND TRACE DIAGRAMS

For definiteness, consider the problem of evaluating the Bloch-Horowitz perturbative expansion of the effective Hamiltonian $\mathscr{H}=H_0+\mathscr{V}$, where H_0 is the independent-particle shell-model Hamiltonian.

The effective interaction $\mathscr{V}$ is expanded in terms of the two-body residual interaction V, as follows:

$$\mathscr{V}=\mathscr{V}^{(1)}+\mathscr{V}^{(2)}+\cdots , \tag{1}$$

where

$$\mathscr{V}^{(n)}=V\left[\frac{Q}{\omega-H_0}V\right]^{n-1} . \tag{2}$$

Here Q is the orthogonal projection on the excluded space (the complement of the model space), H_0 is the single-particle Hamiltonian, and ω is the starting energy.

We use rank-i spherical tensor creation operators A and destruction operators B defined in terms of the conventional operators $a^\dagger$ and a by

$$A^i_\mu=a^\dagger_{i\mu},\quad B^i_\mu=(-1)^{i+\mu}a_{i-\mu} . \tag{3}$$

These definitions imply the following commutation relations in the representation where A and B are coupled to tensorial rank Γ:

$$(A^r\times B^s)^\Gamma+(-1)^{r+s-\Gamma}(B^s\times A^r)^\Gamma=[r]^{1/2}\delta_{\Gamma 0}\delta_{rs} . \tag{4}$$

The two-body interaction can now be written as

$$V=-\tfrac{1}{4}\sum_{rstu\Gamma}[\Gamma]^{1/2}W^\Gamma_{rstu}[(A^r\times A^s)^\Gamma\times(B^t\times B^u)^\Gamma]^0 , \tag{5}$$

where W^Γ_{rstu} are unnormalized antisymmetrized two-body matrix elements of V, related to the normalized matrix elements $\mathscr{W}^\Gamma_{rstu}$, by

$$W^\Gamma_{rstu}\equiv\zeta^{-1}_{rs}\zeta^{-1}_{tu}\mathscr{W}^\Gamma_{rstu} , \tag{6}$$

where

$$\zeta_{ij}\equiv(1+\delta_{ij})^{-1/2} . \tag{7}$$

The superscript Γ represents the total angular momentum including isospin if JT representation is used.

Our problem now is to evaluate matrix elements of $\mathscr{V}^{(n)}$ between states of two particles relative to a closed-shell core. Let the single particle orbits be divided into two groups: the core or hole orbits $c_1,c_2,c_3,\ldots$, and the valence or particle orbits $v_1,v_2,v_3\ldots$. The core state $|c\rangle$ is then the one with all the core orbits fully occupied and valence orbits completely empty. If the core orbits have definite angular momentum, as we assume, $|c\rangle$ will have zero angular momentum, and also zero isospin in appropriate circumstances.

Define a set of pair-creation operators by

$$Z^\Gamma_x=Z^\Gamma_{ij}=-\zeta_{ij}[A^i\times A^j]^\Gamma , \tag{8}$$

and their Hermitian conjugates by

$$\bar{Z}^\Gamma_x=\bar{Z}^\Gamma_{ij}=\zeta_{ij}[B^i\times B^j]^\Gamma , \tag{9}$$

where $x\equiv(i,j)$ denotes the configuration of the pair. Then the normalized two-particle states can be written

$$|\psi^\Gamma_x\rangle=Z^\Gamma_x|c\rangle . \tag{10}$$

We can now express the desired matrix element of the nth order effective interaction $\mathscr{V}^{(n)}$ as the core expectation value of the angular-momentum coupled product of operators, denoted for simplicity by

$$\hat{O}^{(n)}\equiv(\bar{Z}^\Gamma_x\times\mathscr{V}^{(n)}\times Z^\Gamma_y)^0 , \tag{11}$$

unless this results in ambiguity. We have

$$\langle\psi^\Gamma_x|\mathscr{V}^{(n)}|\psi^\Gamma_y\rangle=[\Gamma]^{-1/2}\langle c|\hat{O}^{(n)}|c\rangle , \tag{12}$$

where the factor

$$[\Gamma]^{-1/2}\equiv(2\Gamma+1)^{-1/2} \tag{13}$$

arises from expressing the scalar product of two tensors of rank Γ in terms of their coupling to zero rank.

The evaluation of Eq. (12) of course involves the application of Wick's theorem combined with suitable angular momentum recoupling rules. To show how this problem is connected to that of evaluating configuration traces, we introduce some notation. A configuration is specified by the number of particles in each active orbit. This may be written in vector notation as $\vec{m}=(m_1,m_2,m_3,\ldots)$, where m_i is the number of particles in the ith orbit. We may write $\vec{m}$ as a direct sum of core and valence parts,

$$\vec{m}=(\vec{m}_c,\vec{m}_v) , \tag{14}$$

where $\vec{m}_c=(m_{c_1},m_{c_2},\ldots)$ are the occupancies of the core orbits and $\vec{m}_v=(m_{v_1},m_{v_2},\ldots)$ the occupancies of the valence orbits. Let N_i be the maximum number of particles that can be put into the ith orbit. The number of independent states that can be formed with m_i particles in orbit i is

$$d_i=\binom{N_i}{m_i} , \tag{15}$$

where $\binom{N}{m}$ is the binomial coefficient. The dimensionality of the configuration $\vec{m}$ is

$$d_{\vec{m}}=\binom{\vec{N}}{\vec{m}} , \tag{16a}$$

in terms of the vector binomial coefficient defined by

$$\binom{\vec{N}}{\vec{m}}\equiv\prod_i\binom{N_i}{m_i} . \tag{16b}$$

The configuration trace of an operator $\hat{O}$ is then defined by

$$\langle\!\langle\hat{O}\rangle\!\rangle^{\vec{m}}=\sum_{\alpha\in\vec{m}}\langle\alpha|\hat{O}|\alpha\rangle . \tag{17}$$

The particular configuration $\vec{m}_0\equiv(\vec{N}_c,0)$, with all the core orbits fully occupied ($\vec{m}_c=\vec{N}_c$) and the valence orbits empty ($\vec{m}_v=0$), spans a space of dimension 1 and consists solely of the core state $|c\rangle$. Hence the matrix element of the nth order perturbation term [Eq. (12)] is given by

$$\begin{aligned}\langle\psi^\Gamma_x|\mathscr{V}^{(n)}|\psi^\Gamma_y\rangle&=[\Gamma]^{-1/2}\langle\!\langle(\bar{Z}^\Gamma_x\times\mathscr{V}^{(n)}\times Z^\Gamma_y)^0\rangle\!\rangle^{\vec{m}_0}\\&=[\Gamma]^{-1/2}\langle\!\langle\hat{O}^{(n)}\rangle\!\rangle^{\vec{m}_0} .\end{aligned} \tag{18}$$

Let us return to the study of Eq. (2). We recognize that V is a linear combination of unit scalar two-body operators defined by

$$U(q)\equiv U^\Gamma_{rstu}\equiv-\tfrac{1}{4}[\Gamma]^{1/2}[(A^r\times A^s)^\Gamma\times(B^t\times B^u)^\Gamma]^0 , \tag{19}$$

where $q \equiv (\Gamma rstu)$ stands for the quantum numbers needed to characterize a two-body matrix element. Using also the compact notation

$$W(q) \equiv W^{\Gamma}_{rstu} , \tag{20}$$

we can write

$$V = \sum_{q} W(q) U(q) . \tag{21}$$

In view of Eqs. (2) and (21), the right-hand side of Eq. (11) is essentially a multinomial, i.e., a product of sums, each of the form (21). The following expansion results:

$$\mathscr{V}^{(n)} = \sum_{\vec{q}} \left[\prod_{i=1}^{n} W(q_i) \right] U(q_1) \frac{Q}{e} U(q_2) \cdots \frac{Q}{e} U(q_n) . \tag{22}$$

Here $\vec{q} \equiv (q_1, q_2, \ldots, q_n)$ is one possible set of n q's, each selected from among the values summed over in (21). The operators $Q/e \equiv Q/(\omega - H_0)$ are the propagators; each intermediate state of definite configuration is an eigenstate of Q/e. The Q/e just to the left of $U(q_i)$ gets replaced by its eigenvalue $g(q,i)$, which depends on the intermediate configuration and hence is determined by the set $\{q_{i'}(i' < i)\}$.

Now from Eqs. (18) and (22),

$$\langle \psi^{\Gamma}_x \mid \mathscr{V}^{(n)} \mid \psi^{\Gamma}_y \rangle = [\Gamma]^{-1/2} \sum_{\vec{q}} \left[\prod_{i=1}^{n} W(q_i) g(\vec{q},i) \right] \langle\langle [\bar{Z}^{\Gamma}_x \times U(q_1) \times U(q_2) \times \cdots \times U(q_n) \times Z^{\Gamma}_y]^0 \rangle\rangle^{\vec{m}_0} , \tag{23}$$

where $g(\vec{q},1) = 1$ by convention. Defining

$$D^{(n)\Gamma}_{xy\vec{q}} \equiv \langle\langle [\bar{Z}^{\Gamma}_x \times U(q_1) \times \cdots \times U(q_n) \times Z^{\Gamma}_y]^0 \rangle\rangle^{\vec{m}_0} , \tag{24}$$

we can write

$$\langle \psi^{\Gamma}_x \mid \mathscr{V}^{(n)} \mid \psi^{\Gamma}_y \rangle = [\Gamma]^{-1/2} \sum_{\vec{q}} \left[\prod_{i=1}^{n} W(q_i) g(\vec{q},i) \right] D^{(n)\Gamma}_{xy\vec{q}} . \tag{25}$$

Having expressed the result in terms of the quantity $D^{(n)\Gamma}_{xy\vec{q}}$, we are now ready to exploit the general methods previously developed for the evaluation of configuration traces of angular-momentum-coupled tensor combinations of creation and annihilation operators. The use of Wick's theorem is of course essential to the discussion of (24). To represent each possible type of fully contracted term, Ref. 4 uses a special kind of Hugenholtz diagram which we will call a "trace diagram." As in all Hugenholtz diagrams, each basic operator (e.g., two-body interaction, one-body potential, etc.) is represented by a dot. Each single-particle creation operator in the basic operator is represented by an outgoing line coming from the dot and each annihilation operator by an incoming line. For example, the two-body part of a Hamiltonian is represented by a dot with two outgoing and two incoming lines. The direction of each line is indicated by an arrow, and the contraction between a pair of single particle operators is indicated by a line coming from the creation operator A and going to the annihilation operator B. The basic operators in a diagram are conventionally arranged in vertical order with the leftmost one in the equation on the top. As a result, a "downgoing" line represents a left contraction, i.e., one with the creation operator on the left of the annihilation operator. An "upgoing" line, on the other hand, represents a right contraction, i.e., one with the creation operator on the right. Since the trace may be taken over a configuration $\vec{m}$ that does not in general correspond to a closed core, for trace diagrams there is *no* rule that upgoing (downgoing) lines are restricted to particle (hole) orbits. This is in contrast to the usual diagrams of perturbation theory.

A fundamental general result of Ref. 4 is the "trace equation,"

$$\langle\langle \hat{O} \rangle\rangle^{\vec{m}} = \sum_{\vec{p}\,\vec{t}} \begin{bmatrix} \vec{N} - \vec{p} \\ \vec{m} - \vec{t} \end{bmatrix} \hat{O}^{\vec{p}}_{\vec{t}} , \tag{26}$$

where

$$\hat{O}^{\vec{p}}_{\vec{t}} = \sum_{\kappa} \hat{O}^{\vec{p}}_{\vec{t}}(\kappa) \tag{27}$$

is the sum of all the trace diagrams $\hat{O}^{\vec{p}}_{\vec{t}}(\kappa)$ having a total of p_i contraction lines in the ith orbit with t_i of them downgoing and $(p_i - t_i)$ upgoing. Here κ represents the contraction pattern of each individual diagram.

Let us now consider the application of Eq. (26) in the special case $\vec{m} = \vec{m}_0$, corresponding to the core configuration. We shall show that for this case, upgoing (downgoing) lines in trace diagrams can be restricted to particle (hole) orbits, so that there is a one-to-one correspondence between the trace diagrams and the diagrams of perturbation theory.

The proof follows easily if we consider the fixed particle-rank or hole-rank components of the operator $\hat{O}$ in each orbit. An operator with fixed particle (hole) rank k is one made up of k single-particle creation operators and k annihilation operators, with all the creation operators on the left (right) of the annihilation operators. Therefore, a fully occupied orbit can support only the zero-hole-rank component of $\hat{O}$. Any operator of nonzero hole rank has at least one single-particle creation operator

on the right of all the annihilation operators of the orbit and therefore gives zero when acting on the fully occupied state. Similarly, an empty orbit can support only the zero-particle-rank component of $\hat{O}$ since any nonzero component of $\hat{O}$ has at least one single-particle annihilation operator on the right of the creation operators. Thus for the core configuration trace, where orbits are either fully occupied or empty, the only nonvanishing component of $\hat{O}$ is the part with zero hole rank in all the hole orbits and zero particle rank in all the particle orbits.

By Wick's theorem the zero particle (hole) rank component of an operator in an orbit is equal to the sum of all the possible right (left) contractions of all the single-particle creation and annihilation operators belonging to the orbit. Since a right (left) contraction pair is represented by an upgoing (downgoing) line in the trace diagram, we can conclude that for the core configuration trace, all upgoing lines can be restricted to particle orbits and all the downgoing lines solely to hole orbits. We call this restriction the "perturbation convention."

Returning to Eq. (26), if we restrict the lines according to the perturbation convention, we have $\vec{t}=(\vec{t}_c,0)$, $\vec{p}=(\vec{t}_c,\vec{p}_v)$ and therefore

$$\begin{pmatrix}\vec{N}-\vec{p}\\ \vec{m}_0-\vec{t}\end{pmatrix}=\begin{pmatrix}\vec{N}_c-\vec{p}_c\\ \vec{m}_{0c}-\vec{t}_c\end{pmatrix}\begin{pmatrix}\vec{N}_v-\vec{p}_v\\ \vec{m}_{0v}-\vec{t}_v\end{pmatrix}$$
$$=\begin{pmatrix}\vec{N}_c-\vec{t}_c\\ \vec{N}_c-\vec{t}_c\end{pmatrix}\begin{pmatrix}\vec{N}_v-\vec{p}_v\\ 0-0\end{pmatrix}=1\ . \tag{28}$$

Equation (26) can now be rewritten as

$$\langle\langle\hat{O}\rangle\rangle^{\vec{m}_0}=\sum_{\vec{p}_v\,\vec{t}_c}\hat{O}^{(\vec{t}_c,\vec{p}_v)}_{(\vec{t}_c,0)}\ . \tag{29}$$

Equation (29) shows that the trace diagrams (restricted by the perturbation convention) are in one-to-one correspondence with the perturbation theory Hugenholtz diagrams.

Because of the one-to-one correspondence between trace and perturbation Hugenholtz diagrams of $\mathscr{V}^{(n)}$, we can use the algebraic expressions derived for trace diagrams directly for effective interaction calculations. The various steps to be followed in an effective interaction calculation remain the same except that the tedious job of deriving the equations is now completely delegated to a computer. Furthermore, for trace calculations we have developed further techniques and a computer program by which the equations are translated directly into Fortran codes. As we shall discuss in Sec. III, it is possible with only simple changes to adapt the machine-written codes to the evaluation of effective interaction matrix elements.

III. ALGEBRAIC EVALUATION OF PERTURBATION DIAGRAMS

We now summarize the details of evaluating the configuration trace (24) by the use of Wick's theorem. It is necessary to consider all the possible contractions among the single particle creation and annihilation operators in $\hat{O}^{(n)}$. For the nth order there are $2n+2$ creation operators involved and, consequently, there are $(2n+2)!$ different possible contraction patterns κ (including those containing self-contractions). Not all the possibilities are distinct and those which are topologically equivalent, i.e., those that can be transformed into each other by symmetry considerations, need not be considered separately. We use the following methods to express all the possible diagrams in terms of a much smaller set of simpler diagrams:[4] (a) the two-body matrix-element symmetries implied by Fermi statistics and Hermiticity; (b) the no-self-contraction rule; (c) the use of permutation symmetry among equal or analogous basic operators; and (d) the use of multipole forms for the two-body operators.

We have written the program DIAGRAM (Ref. 5) to list the basic diagrams. This seemingly simple task can be extremely tedious by hand and, for the higher orders, prone to errors since it is hard to be sure that every possibility of generating another topologically distinct diagram is exhausted. Even with a computer it is not practicable to write all the possible contractions (3.6×10^6 of them for $n=4$) first and then discard all the topologically equivalent ones. In the program DIAGRAM[5] we have made good use of a fast pattern recognition procedure to ensure that a complete set of basic diagrams is produced.

The output of DIAGRAM is used by a second program, JT-RECOUPLING (Ref. 5), which converts the diagrams into algebraic expressions by carrying out the actual contractions in the angular momentum coupled representation. Two contracting operators are first brought into adjacent positions by commuting and Racah recoupling before contraction. The recoupling coefficients, phase factors, and weight factors produced in the process are simplified by the use of sum rules whenever possible. In spite of the fact that this is a rigid procedure, one not likely to be followed if the work is to be done by hand, it is a straightforward one which can be carried out efficiently by a computer. Because of this, as we shall see in Sec. III D, we can afford to explore different possibilities to arrive at the simplest final forms.

A. Two-body matrix-element symmetries

Fermi statistics imply

$$W^{\Gamma}_{rstu}=-(-1)^{r+s-\Gamma}W^{\Gamma}_{srtu}=-(-1)^{t+u-\Gamma}W_{rsut}\ , \tag{30}$$

while Hermiticity and time reversal invariance imply

$$W^{\Gamma}_{rstu}=W^{\Gamma}_{turs}\ . \tag{31}$$

The programs can optionally be instructed to recognize diagrams which are related by these symmetries, so that redundancy of coding can be avoided.

B. No-self-contraction rule

Self-contracting a two-body operator produces a lower rank operator. In most applications of effective interaction theory, the contributions of these partially contracted operators are included with the contributions of the one-body insertions. In other cases,[6,7] they are treated via unitary decomposition; the two-body operator is unitarily

decomposed into irreducible parts. The unitary rank ≤ 1 parts are essentially lower rank (<2) operators, consisting of products of number operators and (at most) one-body operators. They are simpler to calculate with than are the original two-body operators, and their role in a diagram is no different from that of lower rank operators. We therefore can ignore self-contracted parts of V and concentrate on irreducible (traceless) two-body operators.

C. Permutations of analogous and equal operators

By *analogous* operators we mean those with similar numbers of creation and annihilation operators, coupled in the same way but perhaps multiplied by different shell-dependent coefficients. All the two-body operators U in Eq. (24) are analogous in this sense. Now consider the application of (27) to (24):

$$D^{(n)\Gamma}_{xy\vec{q}} = \sum_{\kappa} D^{(n)\Gamma}_{xy\vec{q}}(\kappa) , \tag{32}$$

where κ ranges over the contractions possible for the quantum number set q. Each κ corresponds to a diagram. By a *permutation* applied to a diagram we mean a permutation of the operators U with corresponding changes in the contraction patterns; so that, for example, if $U(q_i)$ is on the left of $U(q_j)$, a left contraction between $U(q_i)$ and $U(q_j)$ becomes a right contraction when they are interchanged. We represent all diagrams that are permutations of one another by a single *basic diagram*, and we say all of these diagrams are *generated* from that basic diagram. In nth order perturbation theory the number of basic diagrams is less than the total number of diagrams by a factor $n!$, which is large even if n is only 4. All diagrams that are permutations of a given basic diagram give rise to the same *form* of algebraic expression: the expressions differ only by permutation of the quantum numbers q. This greatly reduces the number of different equations and the amount of coding that needs to be done.

Now consider the effect of a permutation on the contribution of a diagram to a model-space matrix element of $\mathscr{V}^{(n)}$, Eq. (12). The operator $\mathscr{V}^{(n)}$ [defined by Eq. (2)] has $n-1$ *equal* factors $(Q/e)V$. Therefore, subjecting the diagram to any permutation that corresponds to some permutation of these equal factors will leave invariant the *value* of its contribution to the matrix element. The symmetric group S_n on n objects has $n!$ elements. Let G be the largest subgroup of S_n under which the contribution of a given basic diagram is invariant, and let n_G be the number of elements in G. Then by Lagrange's theorem for finite groups,[8] the elements of S_n can be classified into $C_G = n!/n_G$ distinct left cosets, each containing exactly n_G elements. The $n!$ diagrams generated from a given basic diagram can be similarly classified into C_G sets, each consisting of n_G equal diagrams. As a result, the amount of actual computation required to evaluate the set of diagrams generated by a particular basic diagram can be reduced by a factor $n!/C_G = n_G$, which can be an important saving. Accordingly, the program exploits permutation symmetry by automatically distinguishing all classes of equal diagrams. It does this essentially by generating all the $n!$ permuted diagrams and then identifies the classes by sorting.

D. Multipole forms of the interaction

The two-body interaction in a closed (and therefore fully contracted) diagram can be written in either of two multipole forms:

$$V \rightarrow \sum \beta^{\nu}_{rstu}[(A^r \times B^t)^{\nu} \times (A^s \times B^u)^{\nu}]^0 , \tag{33}$$

$$V \rightarrow \sum \beta'^{\nu}_{rstu}[(A^r \times B^u)^{\nu} \times (A^s \times B^t)^{\nu}]^0 . \tag{34}$$

(Though these operators are of course not equal to V, they contribute equivalently to any closed diagram.) The two possible types of cross-coupled matrix elements are given by

$$\beta^{\nu}_{rstu} = \sum_{\Gamma} (-1)^{s+t+\Gamma+\nu}[\Gamma][\nu]^{1/2} \begin{Bmatrix} r & s & \Gamma \\ u & t & \nu \end{Bmatrix} W^{\Gamma}_{rstu} \tag{35}$$

and

$$\beta'^{\nu}_{rstu} = \sum_{\Gamma} (-1)^{s-t+\nu}[\Gamma][\nu]^{1/2} \begin{Bmatrix} r & s & \Gamma \\ t & u & \nu \end{Bmatrix} W^{\Gamma}_{rstu} . \tag{36}$$

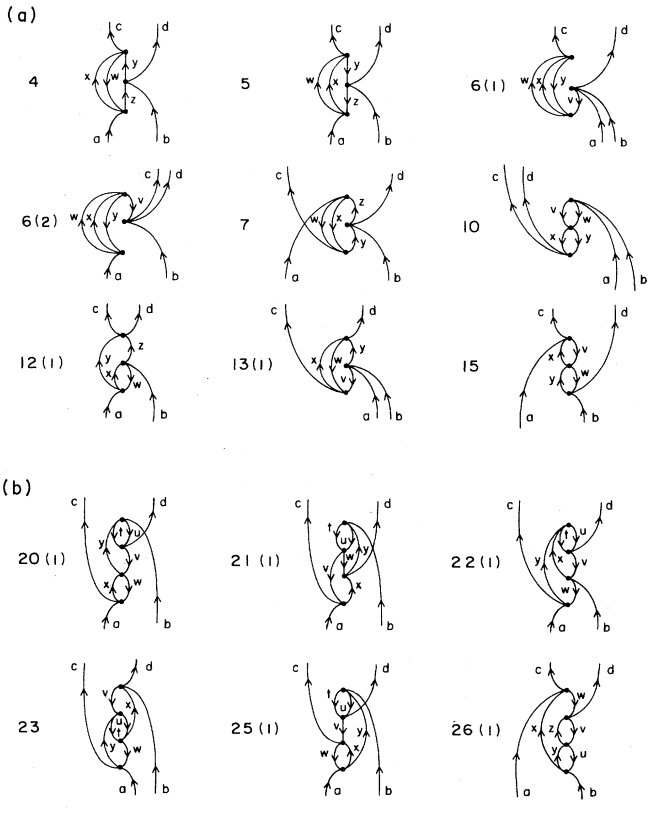

FIG. 1. Basic diagrams of third and fourth orders. (a) shows all third-order basic diagrams. The nonbasic diagram 7 is included to illustrate its relationship to the basic diagram 5, as discussed in the text. (b) shows selected fourth-order basic diagrams.

Reference 2 also makes use of these cross-coupled matrix elements.

Even without going into the details, it is clear that for certain diagrams the *ABAB* form will produce simpler final results. An example of this is the case where the first *B* contracts with an *A* in a basic operator to the left and the second *A* with a *B* to the right. Since the form *AABB* is used in Eq. (5), the same 6-*J* symbol as required to transform from *AABB* to *ABAB* may appear in the intermediate step and, sometimes, in the final result. By absorbing this 6-*J* symbol into the defining matrix elements of the two-body operator, we are likely (but not guaranteed) to produce a final expression with one 6-*J* symbol fewer. In other words, if the multiple form of the defining matrix elements for the operator is used instead of two-body matrix elements, the final expression may be simpler. By allowing the choice of using either W, β, or β' for the defining matrix elements of the V's in Eq. (2) we open up a new degree of freedom to simplify the final expression. However, no way is known to find out *a priori* which one of the three forms is the best for a given diagram. Furthermore, each one of the n V's in Eq. (2) can take a different form independent of the others. We thus have 3^n possibilities that can be explored. With a computer, this is fairly fast and the advantage offered by the increased flexibility can be very rewarding.

IV. DISCUSSION OF RESULTS

The Appendix displays our algebraic results for the third and fourth order diagrams considered by Barrett and Kirson in Ref. 3. Figure 1 shows the corresponding basic diagrams. To make the comparison easier, we adopt Barrett and Kirson's symbols and diagram numbers, and use their simple $2\hbar\omega$ energy denominators. But for simplicity and clarity, we write our results in the neutron-proton (n-p) formalism instead of the isospin formalism employed in Ref. 3. Thus to each of our phases, weights, and recoupling coefficients, one should add an analogous isospin factor, to convert the results to the isospin formalism. These isospin factors can be produced simply by replacing each single-particle angular momentum j and coupled angular momentum J in the angular momentum factors by the isospin t and T, respectively. Of course all matrix elements now need an additional isospin label. For example, the algebraic result for diagram 4 [Eq. (A1)] becomes in isospin formalism

$$\sum_{\substack{wxyz \\ J_1J_2T_1T_2}} (-1)^{j_c+j_d+j_b+j_x+j_w-j_z}[J_2T_2] \begin{Bmatrix} j_c & J_1 & j_y \\ J_2 & j_d & J \end{Bmatrix} \begin{Bmatrix} j_a & J_1 & j_z \\ J_2 & j_b & J \end{Bmatrix} \times \begin{Bmatrix} \frac{1}{2} & T_1 & \frac{1}{2} \\ T_2 & \frac{1}{2} & T \end{Bmatrix} \begin{Bmatrix} \frac{1}{2} & T_1 & \frac{1}{2} \\ T_2 & \frac{1}{2} & T \end{Bmatrix} \frac{\beta'(cwxyJ_1T_1)W(ydzbJ_2T_2)\beta'(xzawJ_1T_1)}{(2\hbar\omega)^2} . \tag{37}$$

We also avoid the normalization factor N_{abcd} of Barrett and Kirson in all the expressions by writing our results for the unnormalized matrix elements of the effective interaction as defined in Eq. (6).

We use an abbreviated notation, in which $\mathscr{V}_p$ is the contribution of diagram p to the matrix element (12). Moreover, only the expressions for the basic diagrams are given explicitly. Instead of giving the expression for a permuted diagram (which can be generated by permutation from a basic diagram), we give only the permutation that relates the diagram to the basic diagram. For example, diagram 7 can be generated by interchanging the first and third V in diagram 5; we then write

$$\mathscr{V}_7 = P(321)\mathscr{V}_5 , \tag{38}$$

where $P(i,j,\ldots)$ denotes the permutation that changes the first V to the ith V, the second V to the jth V, etc. As a result, our equations not only are simpler but also serve to indicate the permutation relations among the diagrams. To produce the explicit expressions for the permuted diagrams, one needs only to permute accordingly all symbols associated with a V, starting from the expression for the basic diagram. For example, the result for diagram 7 can be obtained simply by interchanging (c,y,w,x,J_1) with (w,x,a,z,J_1) in diagram 5. Note, however, these permuted results should not be compared directly with those in Ref. 3 because many of the state lines in the permuted diagrams are renamed in Ref. 3. To be self-contained, we show our basic diagrams in Fig. 1, with state lines named exactly as in Ref. 3. Some of these basic diagrams are related by Hermitian conjugation, as pointed out in Ref. 3.

It is clear by comparing Eqs. (A1)—(A31) with the results of Ref. 3 that all expressions that involve recoupling coefficients are simplified by using the multipole matrix elements. As a consequence, none of our results for the third order diagrams involves more than two 6-*J* symbols and only two involve two 6-*J*'s, three involve one 6-*J*, and three have no 6-*J*. This is much simpler than the results given in Ref. 3 where in the n-p formalism two diagrams would have four 6-*J*'s, three would have one 9-*J*, and three would have no 6-*J*. All the fourth order diagrams considered in Ref. 3 have been simplified as shown in Eqs. (A1)—(A31). As a matter of fact the most complicated fourth order diagram in our complete list involves only five 6-*J* coefficients. More important, probably, is that the number of summation variables is often reduced together with the reduction of the 6-*J* symbols. This is most noticeable in Eqs. (A15) and (A30) for the basic diagrams 15 and 26(1) where the summation variables are three fewer than in the results of Ref. 3.

V. CONCLUSIONS

Computer programs now exist that will perform the Fermion algebra and angular momentum recoupling needed to construct approximate expressions for effective interactions. These may be based either on perturbation theory or on other approximations such as moment theory.[1,6] As a result possible doubts about the reliability and efficiency of expressions for effective-interaction matrix elements need no longer hamper calculations.

In particular, complete expressions for the fourth order effective-interaction matrix elements are now available. Numerical evaluation of these would improve the accuracy of effective interaction calculations, and permit the errors of approximation to be estimated, as shown by Chang and Vincent.[1] However, caution about the practicability of the calculations is needed, because of the large amount of numerical calculation that is required.

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APPENDIX: SELECTED ALGEBRAIC RESULTS

The notation used in the following equations is described in Sec. IV of the main text.

$$\mathscr{V}_4=\sum_{\substack{wxyz\\J_1J_2}}(-1)^{j_c+j_d+j_b+j_x+j_w-j_z}[J_2]\begin{Bmatrix}j_c & J_1 & j_y\\ J_2 & j_d & J\end{Bmatrix}\begin{Bmatrix}j_a & J_1 & j_z\\ J_2 & j_b & J\end{Bmatrix}\frac{\beta'(cwxyJ_1)W(ydzbJ_2)\beta'(xzawJ_1)}{(2\hbar\omega)^2}\,, \tag{A1}$$

$$\mathscr{V}_5=-\tfrac{1}{2}\sum_{\substack{wxyz\\J_1J_2}}(-1)^{j_d-j_z+J+J_1+J_2}[J_1][J_2]^{1/2}\begin{Bmatrix}j_a & j_c & J_z\\ j_y & j_z & J_1\end{Bmatrix}\begin{Bmatrix}j_a & j_c & J_2\\ j_d & j_b & J\end{Bmatrix}\frac{W(cywxJ_1)\beta(zdybJ_2)W(wxazJ_1)}{(2\hbar\omega)^2}\,, \tag{A2}$$

$$\mathscr{V}_{6(1)}=-\frac{1}{2[j_c]}\sum_{vwxyJ_1}\delta_{j_vj_c}[J_1]\frac{W(ycxwJ_1)W(vdabJ)W(xwyvJ_1)}{(2\hbar\omega)^2}\,, \tag{A3}$$

$$\mathscr{V}_{6(2)}=-\frac{1}{2[j_a]}\sum_{vwxyJ_1}\delta_{j_vj_a}[J_1]\frac{W(yvxwJ_1)W(cdvbJ)W(xwyaJ_1)}{(2\hbar\omega)^2}\,, \tag{A4}$$

$$\mathscr{V}_7=P(321)\mathscr{V}_5\,, \tag{A5}$$

$$\mathscr{V}_8=P(321)\mathscr{V}_4\,, \tag{A6}$$

$$\mathscr{V}_{9(1)}=P(321)\mathscr{V}_{6(1)},\quad \mathscr{V}_{9(2)}=P(321)\mathscr{V}_{6(2)}\,, \tag{A7}$$

$$\mathscr{V}_{10}=\tfrac{1}{4}\sum_{vwxy}\frac{W(vwabJ)W(xyvwJ)W(cdxyJ)}{(2\hbar\omega)^2}\,, \tag{A8}$$

$$\mathscr{V}_{11(1)}=P(231)\mathscr{V}_{10},\quad \mathscr{V}_{11(2)}=P(312)\mathscr{V}_{10}\,, \tag{A9}$$

$$\mathscr{V}_{12(1)}=\sum_{wxyzJ_2}(-1)^{j_a+j_w+j_x-j_z}\begin{Bmatrix}j_a & j_b & J\\ j_z & j_y & J_2\end{Bmatrix}\frac{W(cdyzJ)\beta(wzxbJ_2)\beta(yxawJ_2)}{(2\hbar\omega)^2}\,, \tag{A10}$$

$$\mathscr{V}_{12(2)}=-P(132)\mathscr{V}_{13(1)}\,, \tag{A11}$$

$$\mathscr{V}_{13(1)}=-\sum_{vwxyJ_1}(-1)^{j_d+j_v+j_w-j_x+J}\begin{Bmatrix}j_c & j_d & J\\ j_y & j_v & J_1\end{Bmatrix}\frac{\beta(dwyxJ_1)W(vyabJ)\beta(xcwvJ_1)}{(2\hbar\omega)^2}\,, \tag{A12}$$

$$\mathscr{V}_{13(2)}=-P(213)\mathscr{V}_{12(1)}\,, \tag{A13}$$

$$\mathscr{V}_{14(1)}=-P(213)\mathscr{V}_{13(1)},\quad V_{14(2)}=P(312)\mathscr{V}_{12(1)}\,, \tag{A14}$$

$$\mathscr{V}_{15}=\sum_{vwxyJ_1}(-1)^{j_a+j_d+j_v+j_w+j_x+j_y+J+J_1}[J_1]^{-1/2}\begin{Bmatrix}j_a & j_b & J\\ j_d & j_c & J_1\end{Bmatrix}\frac{\beta(cvaxJ_1)\beta(wxyvJ_1)\beta(ydwbJ_1)}{(2\hbar\omega)^2}\,, \tag{A15}$$

$$\mathscr{V}_{16(1)}=P(132)\mathscr{V}_{15},\quad \mathscr{V}_{16(2)}=P(213)\mathscr{V}_{15}\,, \tag{A16}$$

$$\mathscr{V}_{17(1)}=-P(213)\mathscr{V}_4,\quad \mathscr{V}_{17(2)}=-P(132)\mathscr{V}_4\,, \tag{A17}$$

$$\mathscr{V}_{18(1)}=-P(312)\mathscr{V}_4,\quad \mathscr{V}_{18(2)}=-P(231)\mathscr{V}_4\,, \tag{A18}$$

$$\mathscr{V}_{19(1)}=-P(312)\mathscr{V}_5,\quad \mathscr{V}_{19(2)}=-P(231)\mathscr{V}_5\,, \tag{A19}$$

$$\mathscr{V}_{20(1)}=-\tfrac{1}{2}\sum_{tuvwxyJ_1J_2}(-1)^{j_a+j_v+j_w+j_x+J+J_1}[J_1]\begin{Bmatrix} j_a & J_2 & j_c \\ j_d & J & j_b \end{Bmatrix}\begin{Bmatrix} j_d & j_v & J_1 \\ j_y & j_b & J_2 \end{Bmatrix}$$
$$\times\frac{W(tuybJ_1)W(vdtuJ_1)\beta(ywvxJ_2)\beta(cxawJ_2)}{(2\hbar\omega)^2}, \tag{A20}$$

$$\mathscr{V}_{20(2)}=P(3421)\mathscr{V}_{20(1)}, \tag{A21}$$

$$\mathscr{V}_{21(1)}=\tfrac{1}{2}\sum_{tuvwxyJ_1J_2J_3}(-1)^{j_a+j_b+j_d+j_w+j_x+j_y+J+J_1+J_2+J_3}[J_1][J_2][J_3]^{1/2}\begin{Bmatrix} j_a & j_b & J \\ j_d & j_c & J_3 \end{Bmatrix}\begin{Bmatrix} J_1 & J_2 & J_3 \\ j_d & j_b & j_y \end{Bmatrix}\begin{Bmatrix} J_1 & J_2 & J_3 \\ j_x & j_v & j_w \end{Bmatrix}$$
$$\times\frac{W(tuybJ_1)W(vwtuJ_1)W(ydxwJ_2)\beta(cxavJ_3)}{(2\hbar\omega)^3} \tag{A22}$$

$$\mathscr{V}_{21(2)}=-P(3421)\mathscr{V}_{21(1)}, \tag{A23}$$

$$\mathscr{V}_{22(1)}=\tfrac{1}{2}\sum_{tuvwxyJ_1J_2J_3}(-1)^{j_a+j_b+j_d+j_v+j_x+j_y+J+J_1+J_2+J_3}[J_1][J_2][J_3]^{1/2}\begin{Bmatrix} j_a & j_b & J \\ j_d & j_c & J_3 \end{Bmatrix}\begin{Bmatrix} J_1 & J_2 & J_3 \\ j_w & j_y & j_x \end{Bmatrix}\begin{Bmatrix} J_1 & J_2 & J_3 \\ j_b & j_d & j_v \end{Bmatrix}$$
$$\times\frac{W(tuyxJ_1)W(vdtuJ_1)W(wxvbJ_2)\beta(cyawJ_3)}{(2\hbar\omega)^3}, \tag{A24}$$

$$\mathscr{V}_{22(2)}=P(3421)\mathscr{V}_{21(1)}, \tag{A25}$$

$$\mathscr{V}_{23}=-\tfrac{1}{2}\sum_{tuvwxyJ_1J_2}(-1)^{j_a+j_d+j_x+j_y+J+J_2}[J_2]\begin{Bmatrix} j_x & j_w & J_2 \\ j_y & j_v & J_1 \end{Bmatrix}\begin{Bmatrix} j_a & j_b & J \\ j_d & j_c & J_1 \end{Bmatrix}$$
$$\times\frac{\beta(vdxbJ_1)W(tuvyJ_2)W(xwtuJ_2)\beta(cyawJ_1)}{(2\hbar\omega)^3}, \tag{A26}$$

$$\mathscr{V}_{24(1)}=P(2314)\mathscr{V}_{21(1)},\quad \mathscr{V}_{24(2)}=P(2341)\mathscr{V}_{22(1)}, \tag{A27}$$

$$\mathscr{V}_{25(1)}=\tfrac{1}{2}\sum_{tuvwxyJ_1J_2}(-1)^{j_b+j_c+j_d+j_w+j_x-j_y}[J_1]\begin{Bmatrix} J & J_1 & J_2 \\ j_v & j_c & j_d \end{Bmatrix}\begin{Bmatrix} J & J_1 & J_2 \\ j_y & j_a & j_b \end{Bmatrix}$$
$$\times\frac{W(tuybJ_1)W(vdtuJ_1)\beta'(cwxvJ_2)\beta'(xyawJ_2)}{(2\hbar\omega)^3}, \tag{A28}$$

$$\mathscr{V}_{25(2)}=P(3412)\mathscr{V}_{25(1)}, \tag{A29}$$

$$\mathscr{V}_{26(1)}=-\sum_{xyzuvwJ_1J_2}(-1)^{j_a+j_b+j_c+j_u+j_v+j_w+j_y+j_z+J_2}\frac{[J_1]}{[J_2]^{1/2}}\begin{Bmatrix} J & J_1 & J_2 \\ j_w & j_d & j_c \end{Bmatrix}\begin{Bmatrix} J & J_1 & J_2 \\ j_x & j_b & j_a \end{Bmatrix}$$
$$\times\frac{W(cwaxJ_1)\beta'(vdwzJ_2)\beta'(uzvyJ_2)\beta'(xyubJ_2)}{(2\hbar\omega)^3}, \tag{A30}$$

$$\mathscr{V}_{26(2)}=P(4123)\mathscr{V}_{26(1)}. \tag{A31}$$

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