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Contraction theorem for the algebraic reduction of (anti)commutators involving operator strings

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A proof by induction is given of the so-called contraction theorem for the evaluation of (anti)commutators of strings of Fermion creation and annihilation operators. This theorem bears some formal similarity to Wick's theorem but is essentially simpler and its applications do not lead to any disconnected diagrams. Examples of applications to configuration-interaction and coupled-cluster methods are presented.

I. INTRODUCTION

Since the inception of perturbation theory in a second-quantized form, the use of diagrams has greatly alleviated the problem of identifying and formulating the plethora of terms that need consideration. This has been particularly true for high orders of perturbation theory. Central to such diagrammatic enumeration is, of course, the linked-cluster theorem, which states, in effect, that all relevant energy and wave-function terms can be represented by linked diagrams only. Using a list of rules then allows one to "translate" such diagrams into algebraic expressions. This approach has also been adopted by the formulators and users of the coupled-cluster method.[1,2] This method is intimately connected to many-body perturbation theory. Indeed, iteration of the nonlinear equations yields infinite series of perturbation terms all representable by linked diagrams.

The obvious advantage of the use of diagrams is the pictorialization of generally messy algebraic expressions. A disadvantage is some obfuscation of underlying mathematical structure and properties such as analyzed by Živković and Monkhorst[3] in connection with the coupled-cluster method. Other drawbacks are the possibility of overlooking certain diagrams, particularly in high orders of perturbation theory, and the existence of many rules.

In our study and exposition of the configuration-interaction, perturbation, and coupled-cluster methods[4] we found it useful to make extensive use of commutator algebra. This enabled us both to present a systematic way of obtaining equations for these methods and to expose and preserve their underlying structures. The key tool is the so-called contraction theorem, which we wish here to present and rigorously prove by induction. This theorem is formally somewhat similar to the time-independent form of Wick's theorem,[5] but is essentially simpler to apply in practice. Its applications do not require using any diagrams and do not lead to any combinatorial and topological problems. Moreover, this theorem produces expressions which, if interpreted diagrammatically, correspond to connected graphs only.

After a few definitions we proceed to a statement and proof of the contraction theorem. This will be followed by a number of examples from the configuration-interation and coupled-cluster methods.

II. OPERATOR STRINGS, (ANTI)COMMUTATORS, AND CONTRACTIONS

In the following, we will denote by a_μ a Fermion annihilation operator and by a^μ its Hermitian conjugate $a_\mu^\dagger$, also called a creation operator. These operators satisfy the usual anticommutation relations

$$[a_\mu, a_\nu]_+ = [a^\mu, a^\nu]_+ = 0\,, \tag{1}$$

$$[a^\mu, a_\nu]_+ = \delta_{\mu\nu}\,. \tag{2}$$

Definition 1. A *string* of annihilation and/or creation operators is a product of such operators

$$B = b_1 b_2 \cdots b_n\,, \tag{3}$$

where each b_i may be any a^μ or a_μ. Throughout this paper, the Latin subscripts $i, j, \ldots,$ will always indicate positions in strings. These strings can contain the same operator more than once. In that case a reduction can be effected by individual-operator anticommutation to adjacency followed by using the identities

$$\begin{aligned} &a_\mu a_\mu = a^\mu a^\mu = 0\,, \\ &a_\mu a^\mu a_\mu = a_\mu\,, \\ &a^\mu a_\mu a^\mu = a^\mu\,. \end{aligned} \tag{4}$$

We will now consider the commutation or anticommutation of operator strings.

Definition 2. The (anti)commutator $[B,C]_\pm$ of strings $B=b_1b_2\cdots b_n$ and $C=c_1c_2\cdots c_m$ is defined by

$$[B,C]_\pm = BC-(-1)^{nm}CB\,. \tag{5}$$

Since Eqs. (4) do not change the parity of n and m the above definition is independent of the particular representation of the string. It is easy to check that

$$[BC,D]_\pm = B[C,D]_\pm + (-1)^{mk}[B,D]_\pm C\,,$$
$$[B,CD]_\pm = [B,C]_\pm D + (-1)^{nm}C[B,D]_\pm\,, \tag{6}$$

where $D=d_1d_2\cdots d_k$. An operation closely connected with (anti) commutation is the contraction of operators from a string.

Definition 3. The *contraction* of the string $B=b_1b_2\cdots b_n$ with respect to b_i and b_j is defined as the removal of these two operators from the string and the multiplication of the remaining string by $(-1)^{i-j}[b_i,b_j]_+$. Note that $(-1)^{i-j}$ is equal to -1 (or 1) if there is an even (or odd) number of operators between b_i and b_j. We will indicate the contraction by a line connecting the contracted operators from below. Here are some examples:

$$a^r a_\alpha a^\mu a_\nu = -\delta_{r\nu}a_\alpha a^\mu\,, \tag{7}$$

$$a^r a_\alpha a^\mu a_\nu = 0\,. \tag{8}$$

The multiple contractions are defined as a superposition of single contractions. For example,

$$a^r a^s a_\beta a_\alpha a^\lambda a^\sigma a_\nu a_\mu = \delta_{r\nu} a^s a_\beta a_\alpha a^\lambda a^\sigma a_\mu = -\delta_{r\nu}\delta_{s\mu} a_\beta a_\alpha a^\lambda a^\sigma$$
$$= \delta_{r\nu}\delta_{s\mu}\delta_{\alpha\lambda} a_\beta a^\sigma\,. \tag{9}$$

Note that the phase of the second contraction is determined after removal of a^r and a_ν from the original string. It may easily be shown that multiple contractions can be carried out in any order with the same result.

To prove the contraction theorem, it is convenient to consider the set $\{d_\mu\}$ consisting of all creation and annihilation operators. We may assume, e.g., that $a_\mu = d_{2\mu-1}$ and $a^\mu = d_{2\mu}$ for $\mu=1,2,\ldots,M$, where M is the number of one-particle states. The right (anti)commutator of an arbitrary string B with $d_\mu^\dagger$ will be denoted by

$$B^\mu = [B, d_\mu^\dagger]_\pm\,. \tag{10}$$

Analogously, the left (anti)commutator of C with d_μ will be denoted by

$$C_\mu = [d_\mu, C]_\pm\,. \tag{11}$$

By multiple use of Eqs. (6) it is easy to show that

$$B^\mu = \sum_{i=1}^{n} (-1)^{n-i}[b_i, d_\mu^\dagger]_+ b_1\cdots b_{i-1}b_{i+1}\cdots b_n\,, \tag{12}$$

$$C_\mu = \sum_{j=1}^{m} (-1)^{j-1}[d_\mu, c_j]_+ c_1\ldots c_{j-1}c_{j+1}\ldots c_m\,. \tag{13}$$

Multiplying Eq. (12) by Eq. (13) and summing over all d_μ we find that

$$\sum_\mu B^\mu C_\mu = -\sum_{i=1}^{n}\sum_{j=1}^{m} (-1)^{n+j-i}[b_i,c_j]_+ b_1\ldots b_{i-1}b_{i+1}\ldots b_n c_1\ldots c_{j-1}c_{j+1}\ldots c_m\,, \tag{14}$$

where we have made use of the obvious identity

$$\sum_\mu [b_i, d_\mu^\dagger]_+[d_\mu, c_j]_+ = [b_i, c_j]_+\,. \tag{15}$$

It is easy to see that

$$(-1)^{n+j-i}[b_i,c_j]_+ b_1\ldots b_{i-1}b_{i+1}\ldots b_n c_1\ldots c_{j-1}c_{j+1}\ldots c_m$$

is just the result of a single contraction of the i th and $(n+j)$th elements from the string BC. Thus the right-hand side of Eq. (14) is the negative of all nm possible single contractions of operators, one from the string B and the other from the string C. Introducing the notation

$$\underset{\sqcup}{BC} = \sum_{i=1}^{n}\sum_{j=1}^{m} b_1\cdots b_i\cdots b_n c_1\cdots c_j\cdots c_m \tag{16}$$

we may rewrite Eq. (14) as

$$\underset{\sqcup}{BC} = -\sum_\mu B^\mu C_\mu\,. \tag{17}$$

Analogously, the sum of all double contractions can be written as

$$\underset{\sqcup\!\sqcup}{BC} = \sum_{\mu<\nu} B^{\mu\nu}C_{\mu\nu}\,, \tag{18}$$

where $B^{\mu\nu}$ and $C_{\mu\nu}$ are double (anti)commutators $B^{\mu\nu}=(B^{\mu})^{\nu}$, $C_{\mu\nu}=(C_{\mu})_{\nu}$ and the symbol $\underset{\sqcup\!\sqcup}{BC}$ is defined precisely as

$$\underset{\sqcup\!\sqcup}{BC} = \sum_{i<i'}^{n} \sum_{j\neq j'}^{m} b_1 \cdots b_i \cdots b_{i'} \cdots b_n c_1 \cdots c_j \cdots c_{j'} \cdots c_m \,. \tag{19}$$

To prove Eq. (18), we use the fact that

$$\begin{aligned} B^{\mu\nu} &= -B^{\nu\mu}\,, \\ C_{\mu\nu} &= -C_{\nu\mu}\,, \end{aligned} \tag{20}$$

and expand the double (anti)commutators using Eqs. (12), (13), and (15)

$$\begin{aligned} \sum_{\mu<\nu} B^{\mu\nu}C_{\mu\nu} &= \tfrac{1}{2}\sum_{\nu}\sum_{\mu}(B^{\mu})^{\nu}(C_{\mu})_{\nu} \\ &= -\tfrac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{m}(-1)^{n+j-i}[b_i, c_j]_{+}\sum_{\nu}(b_1\cdots b_{i-1}b_{i+1}\cdots b_n)^{\nu}(c_1\cdots c_{j-1}c_{j+1}\cdots c_m)_{\nu}\,. \end{aligned}$$

Applying now Eq. (17), we immediately arrive at (18). (The factor $\frac{1}{2}$ disappears since the summation in (19) is limited to $i<i'$.) It is not difficult to generalize the above argument and to show that

$$(-1)^k \sum_{\mu_1<\cdots<\mu_k} B^{\mu_1\cdots\mu_k}C_{\mu_1\cdots\mu_k} \tag{21}$$

is equal to the sum of all possible k-tuple contractions of B and C. Symbolically this may be written as

$$\underset{\sqcup\,\vdots\,\sqcup\, k}{BC} = (-1)^k \sum_{\mu_1<\cdots<\mu_k} B^{\mu_1\cdots\mu_k}C_{\mu_1\cdots\mu_k}\,, \tag{22}$$

where the left-hand side is defined precisely as the natural generalization of Eqs. (16) and (19).

III. THE CONTRACTION THEOREM

We are now ready to introduce and prove the central theorem of this paper, namely the contraction theorem. Generally speaking, this theorem enables us to express an (anti)commutator of two strings in terms of all possible single, double, triple, etc. contractions of pairs of operators, one from the string B, the other from the string C. Symbolically this can be written in the following form

$$[B,C]_{\pm} = -\underset{\sqcup}{BC} - \underset{\sqcup\!\sqcup}{BC} - \underset{\sqcup\!\sqcup\!\sqcup}{BC} - \cdots \tag{23}$$

because of Eq. (22), the contraction theorem may be also written in a different, somewhat more algebraic form:

$$[B,C]_{\pm} = \sum_{\mu} B^{\mu}C_{\mu} - \sum_{\mu<\nu} B^{\mu\nu}C_{\mu\nu} + \sum_{\mu<\nu<\lambda} B^{\mu\nu\lambda}C_{\mu\nu\lambda} - \cdots\,. \tag{24}$$

Equation (23) is an easy, mnemonic form of this theorem, whereas Eq. (24), because of its explicit algebraic structure, is convenient for a proof by induction.

Assuming $B=b$, i.e., B consists of a single operator, and C is a string of arbitrary length, we can verify the contraction theorem for the special case where Eq. (24) terminates after just one term:

$$[b,C]_{\pm} = [b,b^{\dagger}]_{+}[b,C]_{\pm} = \sum_{\mu}[b,d_{\mu}^{\dagger}]_{+}C_{\mu}\,. \tag{25}$$

The last equality holds because the only nonvanishing term comes from $d_{\mu}=b$. Since b is a string of length 1, the right-hand side of Eq. (24) reduces to the first term. We have therefore verified the contraction theorem for a string B of length 1.

Next we will show that, if Eq. (24) is satisfied for strings B of length n ($n\geq 1$) it will also be satisfied for strings B of length $n+1$. We write such a string as $B=bD$, where D is of length n. Using Eq. (6) it can easily be verified that

$$[B,C]_{\pm} = [bD,C]_{\pm} = b[D,C]_{\pm} + (-1)^n D[b,C]_{\pm} + (-1)^{n+1}[D,[b,C]_{\pm}]_{\pm}\,. \tag{26}$$

Assuming that $d_1=b$, we can write

$$[b,C]_{\pm} = C_1\,, \tag{27}$$

and consequently

$$[B,C]_{\pm} = b[D,C]_{\pm} + (-1)^n DC_1 + (-1)^{n+1}[D,C_1]_{\pm}\,. \tag{28}$$

When now applying Eq. (24) to above commutators involving D (which is of length n and hence currently assumed valid) we get

$$[B,C]_\pm = b\Big(\sum_\mu D^\mu C_\mu - \sum_{\mu<\nu} D^{\mu\nu}C_{\mu\nu} + \cdots\Big)$$
$$+ (-1)^n D C_1 + (-1)^{n+1}\Big(\sum_\mu D^\mu C_{1\mu} - \sum_{\mu<\nu} D^{\mu\nu} C_{1\mu\nu} + \cdots\Big). \tag{29}$$

We next rewrite Eq. (29) so as to expose the terms with $\mu = 1$, and group the terms in a special manner:

$$[B,C]_\pm = [bD^1 + (-1)^n D]C_1 + \sum_{\mu>1} bD^\mu C_\mu - \sum_\nu [bD^{1\nu} + (-1)^n D^\nu]C_{1\nu} - \sum_{\mu<\nu\ (\mu,\nu>1)} bD^{\mu\nu}C_{\mu\nu}$$
$$+ \sum_{\mu<\nu} [bD^{1\mu\nu} + (-1)^n D^{\mu\nu}]C_{1\mu\nu} + \sum_{\mu<\nu<\lambda\ (\mu,\nu,\lambda>1)} bD^{\mu\nu\lambda}C_{\mu\nu\lambda} - \cdots . \tag{30}$$

We see therefore that $[B,C]_\pm$ can be written as

$$[B,C]_\pm = \sum_l A_l , \tag{31}$$

where the general term A_l can be expressed as the sum of two sums,

$$A_l = (-1)^{l+1}\Big(\sum_{\mu_2<\cdots<\mu_2} [bD^{1\mu_2\cdots\mu_l} + (-1)^n D^{\mu_2\cdots\mu_l}]C_{1\mu_2\cdots\mu_l}$$
$$+ \sum_{\mu_1<\cdots<\mu_l\ (\mu_1,\ldots,\mu_l>1)} bD^{\mu_1\mu_2\cdots\mu_l} C_{\mu_1\mu_2\cdots\mu_l}\Big). \tag{32}$$

With the help of Eq. (26) we now observe that

$$B^1 = [bD, b^\dagger]_\pm = bD^1 + (-1)^n D . \tag{33}$$

Similarly, for $\mu_1, \mu_2, \ldots, \mu_l > 1$ we have

$$B^{1\mu_2\cdots\mu_l} = bD^{1\mu_2\cdots\mu_l} + (-1)^n D^{\mu_2\cdots\mu_l} , \tag{34}$$

$$bD^{\mu_1\mu_2\cdots\mu_l} = (bD)^{\mu_1\mu_2\cdots\mu_l} = B^{\mu_1\mu_2\cdots\mu_l} . \tag{35}$$

Using Eqs. (33)–(35) in Eq. (32) we finally obtain

$$A_l = (-1)^{l+1} \sum_{\mu_1<\cdots<\mu_l} B^{\mu_1\cdots\mu_l} C_{\mu_1\cdots\mu_l} . \tag{36}$$

This completes the proof.

IV. EXAMPLES

We will consider applications of increasing complexity. We start with a selection relevant for our exposition of the configuration-interaction method.[4] Let H_0 be the zeroth-order Hamiltonian given by

$$H_0 = \sum_\mu \epsilon_\mu a^\mu a_\mu \tag{37}$$

and let C_1, C_2, etc., stand for operators that create one, two, etc., particle-hole pairs. If we designate unoccupied states by $r, s, \ldots$ and occupied states by $\alpha, \beta, \ldots$ then such operators can be expressed as

$$C_1 = \sum_{r\alpha} c^r_\alpha a^r a_\alpha ,$$
$$C_2 = \tfrac{1}{4} \sum_{rs,\alpha\beta} c^{rs}_{\alpha\beta} a^r a^s a_\beta a_\alpha , \tag{38}$$

etc. We have occasion to evaluate the commutator of H_0 and C_n. For example,

$$[H_0, C_1] = -[C_1, H_0]$$
$$= \sum_{\substack{r\alpha\\ \mu}} c^r_\alpha \epsilon_\mu (a^r \underline{a_\alpha a^\mu} a_\mu + \underline{a^r a_\alpha a^\mu a_\mu}) . \tag{39}$$

No multiple contractions occur since μ cannot be simultaneously an r and α. The result is

$$[H_0, C_1] = \sum_{r\alpha} c^r_\alpha (-\epsilon_\alpha a^r a_\alpha - \epsilon_r a_\alpha a^r)$$
$$= \sum_{r\alpha} c^r_\alpha (\epsilon_r - \epsilon_\alpha) a^r a_\alpha . \tag{40}$$

Generalization to higher particle-hole excitation operators gives

$$[H_0, C_n] = \Big(\frac{1}{n!}\Big)^2 \sum_{rs\ldots,\alpha\beta\ldots} c^{rs\cdots}_{\alpha\beta\cdots} (\epsilon_r + \epsilon_s + \cdots - \epsilon_\alpha - \epsilon_\beta - \cdots) a^r a^s \ldots a_\beta a_\alpha . \tag{41}$$

We next consider the one-electron operator

$$U=\sum_{\lambda\sigma}\langle\lambda|u|\sigma\rangle\, a^{\lambda}a_{\sigma} \tag{42}$$

for which the contraction with C_1 is

$$[U,C_1]=-[C_1,U]=\sum_{\substack{r\alpha\\ \lambda\sigma}} c^r_\alpha\langle\lambda|u|\sigma\rangle\left(a^r\underline{a_\alpha a^\lambda}a_\sigma+\underline{a^r a_\alpha a^\lambda a_\sigma}+\underline{a^r\underline{a_\alpha a^\lambda}a_\sigma}\right). \tag{43}$$

Since U contains off-diagonal terms, with strings of two operators, only up to double contractions are found. Performing the indicated contractions, we get

$$[U,C_1]=-\sum_{r\alpha\sigma}c^r_\alpha\langle\alpha|u|\sigma\rangle\, a^r a_\sigma-\sum_{r\alpha\lambda}c^r_\alpha\langle\lambda|u|r\rangle\, a_\alpha a^\lambda+\sum_{r\alpha}c^r_\alpha\langle\alpha|u|r\rangle\ . \tag{44}$$

It is now instructive to apply Eq. (44) to the reference state with respect to which particle-hole excitations are defined. If that state is denoted by Φ, and is given by

$$\Phi=\prod_\alpha a^\alpha|0\rangle\ , \tag{45}$$

with $|0\rangle$ the vacuum state, then excited states can be conveniently expressed as

$$\Phi^{rs\cdots}_{\alpha\beta\cdots}=a^r a^s\ldots a_\beta a_\alpha\Phi\,. \tag{46}$$

As a result, upon changing summation indices, we can write

$$[U,C_1]\Phi=\sum_{r\alpha}\left(-\sum_\beta\langle\beta|u|\alpha\rangle c^r_\beta+\sum_s\langle r|u|s\rangle c^s_\alpha\right)\Phi^r_\alpha+\sum_{r\alpha}c^r_\alpha\langle\alpha|u|r\rangle\Phi\,. \tag{47}$$

The commutator of C_2 and U is slightly more involved:

$$\begin{aligned}[U,C_2]=-[C_2,U]=\tfrac{1}{4}\sum_{\substack{rs\alpha\beta\\ \lambda\sigma}} c^{rs}_{\alpha\beta}\langle\lambda|u|\sigma\rangle\Big(&\{a^r a^s a_\beta\underline{a_\alpha a^\lambda}a_\sigma+a^r a^s\underline{a_\beta a_\alpha a^\lambda}a_\sigma\}\\ &+\{a^r\underline{a^s a_\beta a_\alpha a^\lambda a_\sigma}+\underline{a^r a^s a_\beta a_\alpha a^\lambda a_\sigma}\}\\ &+\{a^r\underline{a^s a_\beta\underline{a_\alpha a^\lambda}a_\sigma}+\underline{a^r a^s a_\beta\underline{a_\alpha a^\lambda}a_\sigma}+a^r\underline{a^s\underline{a_\beta a_\alpha a^\lambda}a_\sigma}+\underline{a^r a^s\underline{a_\beta a_\alpha a^\lambda}a_\sigma}\}\Big).\end{aligned} \tag{48}$$

Considerable simplifications occur if we assume that the $c^{rs}_{\alpha\beta}$ are antisymmetric under particle or hole index interchanges:

$$c^{rs}_{\alpha\beta}=-c^{sr}_{\alpha\beta}=-c^{rs}_{\beta\alpha}\,. \tag{49}$$

This can be done without loss of generality in configuration-interaction-type calculations. With this property all terms in Eq. (48) grouped within a pair of curly brackets are identical. Now applying also this equation to Φ, one obtains, after some algebra,

$$[U,C_2]\Phi=\tfrac{1}{2}\sum_{rs,\alpha\beta}\left(-\sum_\gamma\langle\gamma|u|\alpha\rangle c^{rs}_{\gamma\beta}+\sum_p\langle r|u|p\rangle c^{ps}_{\alpha\beta}\right)\Phi^{rs}_{\alpha\beta}+\sum_{rs,\alpha\beta}\langle\alpha|u|r\rangle c^{rs}_{\alpha\beta}\Phi^s_\beta\,. \tag{50}$$

It is straightforward to derive contractions with a two-electron operator. Eight distinct terms appear. When applied to Φ three such terms give rise to two terms each. Therefore the application to Φ contains eleven distinct terms.[4] For an explicit expression we refer to our paper describing the use of the contraction theorem in connection with finite-order perturbation theory.[6]

We will now consider multiple-string contractions. Such contractions arise naturally in the coupled-cluster (CC) method, and the use of the contraction theorem makes it easy to obtain the working equations. In order to motivate the next examples it is useful to summarize the essential features of the CC method. The correlated wave function is expressed as[1,2]

$$\Psi=e^T\Phi\,, \tag{51}$$

where the so-called cluster operator T is given by

$$T=T_1+T_2+\cdots\,, \tag{52}$$

$$T_1=\sum_{r\alpha}t^r_\alpha\, a^r a_\alpha\,, \tag{53}$$

$$T_2=\frac{1}{4}\sum_{rs,\alpha\beta}t^{rs}_{\alpha\beta}\,a^r a^s a_\beta a_\alpha\,, \tag{54}$$

etc. Φ is an eigenfunction of H_0, and Ψ is sought to satisfy the Schrödinger equation with Hamiltonian H given by

$$H = H_0 + U + V\,. \tag{55}$$

U is the one-particle operator of Eq. (42), and V is the two-particle operator responsible for the correlation problem,

$$V = \tfrac{1}{4} \sum_{\mu\nu\lambda\sigma} \langle \mu\nu | v | \lambda\sigma \rangle\, a^{\mu} a^{\nu} a_{\sigma} a_{\lambda}\,. \tag{56}$$

T_1 can be interpreted as an operator that "relaxes" the one-particle states in Φ under the influence of the perturbation $(U+V)$. T_2, T_3, etc., are two-, three-, etc. particle cluster operators that describe the correction in Ψ due to the single and multiple clustering of two, three, etc. particles without explicit correlation between such clusters. For a discussion of the numerous attributes of the CC method as an attractive many-body approach we refer elsewhere.[4] Here we wish to sketch the key steps that are taken to arrive at the equations for the $t_{\alpha\beta\cdots}^{rs\cdots}$ amplitudes of the cluster operators.

The Schrödinger equation can be written

$$He^{T}\Phi = Ee^{T}\Phi\,. \tag{57}$$

Noting that the inverse of $\exp(T)$ is simply $\exp(-T)$ we can equivalently write

$$e^{-T}He^{T}\Phi = E\,\Phi\,. \tag{58}$$

Since $\exp(T)$ is not unitary, the operator on the left-hand side is a non-Hermitian, similarity-transformed Hamiltonian. Because T only creates particle-hole pairs, and because H contains only one- and two-particle operators, this operator is expressible as a *finite* commutator series:

$$\begin{aligned} e^{-T}He^{T} = H &+ [H, T] + \tfrac{1}{2}[[H, T], T] \\ &+ \frac{1}{3!}[[[V, T], T], T] \\ &+ \frac{1}{4!}[[[[V, T], T], T], T]\,. \end{aligned} \tag{59}$$

Termination after a quadruple commutator arises because V contains strings of no more than four operators. An equation for the energy E is obtained by projecting Eq. (58) against Φ. Equations for $t_{\alpha\beta\cdots}^{rs\cdots}$ are obtained by projecting this equation, against $\Phi_{\alpha\beta\cdots}^{rs\cdots}$.[4] In practice one always truncates Eq. (52), usually after the second term, and only projections against those configurations consistent with the $t_{\alpha\beta\cdots}^{rs\cdots}$ kept are included. The marvel of the CC method is that a severe truncation seems to work very well in widely different systems such as the electron gas, nuclei, atoms, and molecules (see, for example, Kümmel *et al.*[7] on nuclear calculations, and Bartlett *et al.*[8] on molecular correlation energy work).

With the contraction theorem, the commutators in Eq. (59) can now be evaluated. Let us consider for example $[[U, T_1], T_1]$:

$$\begin{aligned} [[U, T_1], T_1] &= [T_1 [T_1, U]] \\ &= \sum_{s\beta} t_{\beta}^{s} \Big\{ -\sum_{r\alpha\sigma} t_{\alpha}^{r} \langle \alpha | u | \sigma \rangle \underbrace{a^{s} a_{\beta} a^{r}} a_{\sigma} \\ &\quad - \sum_{r\alpha\lambda} t_{\alpha}^{r} \langle \lambda | u | r \rangle a^{s} \underbrace{a_{\beta} a_{\alpha}} a^{\lambda} \Big\} \end{aligned} \tag{60}$$

(we only show the nonzero terms). Executing the contractions indicated we obtain

$$\begin{aligned} [[U, T_1], T_1] = &\sum_{rs,\alpha\beta} t_{\alpha}^{r} t_{\beta}^{s} \langle \alpha | u | s \rangle\, a_{\beta} a^{r} \\ &- \sum_{rs,\alpha\beta} t_{\alpha}^{r} t_{\beta}^{s} \langle \beta | u | r \rangle\, a^{s} a_{\alpha}\,. \end{aligned} \tag{61}$$

But we recognize that the two sums are identical. Consequently we can express the effect of the double commutator on Φ as

$$\tfrac{1}{2}[[U, T_1], T_1] = \sum_{rs,\alpha\beta} t_{\alpha}^{s} t_{\beta}^{r} \langle \beta | u | s \rangle\, \Phi_{\alpha}^{r}\,. \tag{62}$$

Triple and quadruple contractions involving U vanish, because it contains strings with two operators only. For examples involving V we again refer to the subsequent paper,[6] in which the contraction theorem is applied to order-by-order perturbation theory.

V. RELATION TO WICK'S THEOREM

We wish to point out that the (anti)commutator $[B, C]_{\pm}$ can be cast in a form that exploits Wick's theorem. Starting from Eq. (5) this theorem can be directly applied to strings BC and CB separately.[5] But then the resulting sum of normal (n) products with modified contractions as defined in Ref. 5 involves quite complicated contraction patterns. In forming $[B, C]_{\pm}$ according to Eq. (5) the n products without contractions cancel. However, if B and C are not both normal ordered, combinations of contractions between B and C elements and of elements within the B and C strings occur. Therefore a direct application of Wick's theorem is operationally more involved. Of course, the contraction theorem does not yield operator strings in n-product form. If such forms are desired Wick's theorem can be invoked after one or more applications of the contraction theorem.

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