

Algebra for fermions with a new exclusion principle

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Abstract. We construct the algebra of the creation and destruction operators for spin $\frac{1}{2}$ particles obeying a new exclusion principle which is "more exclusive" than Pauli's exclusion principle: an orbital state shall not contain more than one particle, whether spin up or spin down. The consequences of this algebra are studied and applications to the Hubbard model in condensed matter physics are indicated.

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1. Introduction

Pauli's exclusion principle plays a fundamental role in present-day physics. In this paper, we envisage a quantum-mechanical system of spin $\frac{1}{2}$ particles satisfying a new exclusion principle which is more exclusive than Pauli's principle and which allows the occupation of a single particle (either spin up or down) in any orbital state but forbids the occupation of both spin up and down in the same orbital state. Is it possible to describe such a system consistently using creation and destruction operators? What is the algebra satisfied by such operators? We show that the answer to the first question is in the affirmative and obtain the algebra satisfied by the new creation and destruction operators.

Our work was originally motivated by the Hubbard model in the $U \rightarrow \infty$ limit, which has become a focal point of interest in recent work on high T_c superconductivity. Hubbard model is described by the Hamiltonian

$$H = -t \sum_{\langle ij \rangle} c_{j\alpha}^\dagger c_{i\alpha} + U \sum_i c_{i\sigma}^\dagger c_{i\sigma} c_{i\bar{\sigma}}^\dagger c_{i\bar{\sigma}}$$

where $c_{i\alpha}$ and $c_{i\alpha}^\dagger$ are the annihilation and creation operators for electrons at site i and spin α (either spin up σ or spin down $\bar{\sigma}$). The second term with positive U describes the Coulomb repulsion of the electrons on the same site and in the limit of infinite U it forbids more than one electron on the same site. Although this is the motivation for the new exclusion principle, it will become clear that our results may be of more general interest.

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Section 2 contains the main result of this paper namely the new algebra. Subsequent sections are devoted to the various ramifications of this algebra and show how the algebra describes the system of particles in a consistent manner although the particles do have strange properties. Section 6 contains some physical applications while the final section gives a summary and discussion. In Appendix 1 explicit representations for the new creation and destruction operators are given while Appendix 2 gives the complete set of rules for forming the normal product and the Wick expansion for the operators of the new algebra.

2. The new algebra

We denote by $c_{k\sigma}$ and $c_{k\bar{\sigma}}$ the destruction operators for particles in the orbital state k with spin up and down (σ and $\bar{\sigma}$) and by their hermitian conjugates $c_{k\sigma}^\dagger$ and $c_{k\bar{\sigma}}^\dagger$ the corresponding creation operators. Then, we obtain the following two types of algebras satisfied by them:

Algebra I

$$c_{k\sigma}c_{m\bar{\sigma}} + (1 - \delta_{km})c_{m\bar{\sigma}}c_{k\sigma} = 0 \quad (1)$$

$$c_{k\sigma}c_{m\bar{\sigma}}^\dagger + (1 - \delta_{km})c_{m\bar{\sigma}}^\dagger c_{k\sigma} = 0 \quad (2)$$

$$c_{k\sigma}c_{m\sigma}^\dagger + c_{m\sigma}^\dagger c_{k\sigma} = \delta_{km}(1 - c_{k\bar{\sigma}}^\dagger c_{k\bar{\sigma}}) \quad (3)$$

$$\{c_{k\sigma}, c_{m\sigma}\} = 0 \quad (4)$$

together with all the relations obtained from these by interchanging σ and $\bar{\sigma}$ or by taking hermitian conjugate.

Algebra II

$$c_{k\sigma}c_{m\bar{\sigma}} + c_{m\sigma}c_{k\bar{\sigma}} = 0 \quad (5)$$

$$c_{k\sigma}c_{m\bar{\sigma}}^\dagger = 0 \quad (6)$$

$$c_{k\sigma}c_{m\sigma}^\dagger + c_{m\sigma}^\dagger c_{k\sigma} + c_{m\bar{\sigma}}^\dagger c_{k\bar{\sigma}} = \delta_{km} \quad (7)$$

$$\{c_{k\sigma}, c_{m\sigma}\} = 0 \quad (8)$$

and all the relations obtained from these by interchanging σ and $\bar{\sigma}$ or by taking hermitian conjugate. Algebra II can also be written in the more compact form

$$c_{m\alpha}c_{k\beta}^\dagger = \delta_{\alpha\beta} \left(\delta_{mk} - \sum_{\gamma} c_{k\gamma}^\dagger c_{m\gamma} \right) \quad (9)$$

$$c_{k\alpha}c_{m\beta} + c_{m\alpha}c_{k\beta} = 0 \quad (10)$$

where α, β, γ go over $\sigma, \bar{\sigma}$.

Either of these two algebras can be used to describe the system of spin $\frac{1}{2}$ particles obeying the super-exclusion principle or extended Pauli principle formulated above. Whereas algebra I is inhomogeneous in the orbital indices k and m , algebra II is homogeneous in these indices. One can see that these two algebras differ only for

$k \neq m$. If we consider only a single orbital state (whose label can be suppressed), both these algebras reduce to the following common algebra:

$$c_{\sigma}c_{\bar{\sigma}} = 0 \quad (11)$$

$$c_{\sigma}c_{\bar{\sigma}}^{\dagger} = 0 \quad (12)$$

$$c_{\sigma}c_{\sigma}^{\dagger} = c_{\bar{\sigma}}c_{\bar{\sigma}}^{\dagger} = 1 - c_{\sigma}^{\dagger}c_{\sigma} - c_{\bar{\sigma}}^{\dagger}c_{\bar{\sigma}} \quad (13)$$

$$c_{\sigma}c_{\sigma} = 0 \quad (14)$$

and all the relations obtained from these by interchanging σ and $\bar{\sigma}$ or by taking hermitian conjugate.

Let us first consider the simpler algebra given in eqs (11)–(14). The hermitian conjugate of (14) implements the usual Pauli principle while the hermitian conjugate of (11) implements the extended Pauli principle. The vector space here is 3-dimensional, spanning the three independent ket vectors $|0\rangle$, $|\sigma\rangle$ and $|\bar{\sigma}\rangle$ which denote the vacuum state, the particle state with spin σ and the particle state with spin $\bar{\sigma}$ respectively. Either using these kets and the corresponding bra vectors $\langle 0|$, $\langle \sigma|$, $\langle \bar{\sigma}|$ or by using 3×3 matrices, one can show that (11)–(14) follow (See Appendix 1). In fact, the explicit construction of the 3×3 matrices proves the consistency and completeness* of the algebra defined by eqs (11)–(14).

It may be noted that the operators $c_{\sigma}^{\dagger}c_{\bar{\sigma}}$ and $c_{\bar{\sigma}}^{\dagger}c_{\sigma}$ do not occur in the algebra (eqs (11)–(14)). They are actually spin-flip operators and generate the SU(2) algebra. Defining

$$s_{+} = c_{\sigma}^{\dagger}c_{\bar{\sigma}} \quad (15)$$

$$s_{-} = c_{\bar{\sigma}}^{\dagger}c_{\sigma} \quad (16)$$

$$s_z = \frac{1}{2}(c_{\sigma}^{\dagger}c_{\sigma} - c_{\bar{\sigma}}^{\dagger}c_{\bar{\sigma}}) \quad (17)$$

and using eqs (11)–(14), it is easy to verify the usual SU(2) algebra:

$$[s_{+}, s_{-}] = 2s_z \quad (18)$$

$$[s_{\pm}, s_z] = \mp s_{\pm}. \quad (19)$$

Thus our modification of the usual fermionic anticommutation relations is consistent with invariance under the spin rotations.

With the orbital states included, we get the two types of algebras I and II. These algebras are obtained by extending the arguments of Appendix 1 to the case of two or more number of sites. Algebra I results if we demand total antisymmetry of the wave function for interchange of orbital and spin indices. Algebra II is obtained if we require the validity of (11)–(14) for any linear combinations of orbital states. The motivation for such a requirement is the resulting invariance under unitary transformations discussed below.

* By completeness, we mean that the algebraic relations (11)–(14) define the operators c_{σ} and $c_{\bar{\sigma}}$ and their hermitian conjugates completely.

Antisymmetrisation is obvious if we re-write (1)–(4) for $k \neq m$:

$$c_{k\sigma}c_{m\bar{\sigma}} + c_{m\bar{\sigma}}c_{k\sigma} = 0 \quad (20)$$

$$c_{k\sigma}c_{m\bar{\sigma}}^\dagger + c_{m\bar{\sigma}}^\dagger c_{k\sigma} = 0 \quad (21)$$

$$c_{k\sigma}c_{m\sigma}^\dagger + c_{m\sigma}^\dagger c_{k\sigma} = 0 \quad (22)$$

$$c_{k\sigma}c_{m\sigma} + c_{m\sigma}c_{k\sigma} = 0. \quad (23)$$

In fact, for $k \neq m$, algebra I is identical to the usual algebra for fermions. In contrast, algebra II for $k \neq m$ reads:

$$c_{k\sigma}c_{m\bar{\sigma}} + c_{m\sigma}c_{k\bar{\sigma}} = 0 \quad (24)$$

$$c_{k\sigma}c_{m\bar{\sigma}}^\dagger = 0 \quad (25)$$

$$c_{k\sigma}^\dagger c_{m\sigma} + c_{m\sigma}^\dagger c_{k\sigma} + c_{k\bar{\sigma}}^\dagger c_{m\bar{\sigma}} = 0 \quad (26)$$

$$c_{k\sigma}c_{m\sigma} + c_{m\sigma}c_{k\sigma} = 0. \quad (27)$$

The positions of σ and $\bar{\sigma}$ in (24) must be particularly noted. Whereas (20) implies total antisymmetry for the wave function, (24) implies antisymmetry in the spatial labels only, with the order of the spin indices frozen.

The complete algebra II given in (5)–(8) is invariant under the unitary transformation:

$$d_{r\sigma} = \sum_k U_{rk} c_{k\sigma} \quad (28)$$

$$d_{r\bar{\sigma}} = \sum_k U_{rk} c_{k\bar{\sigma}} \quad (29)$$

where

$$UU^\dagger = U^\dagger U = 1. \quad (30)$$

It is easily seen that the relations of algebra I (eqs (1–4)) are *not* invariant under these unitary transformations because of the terms inhomogeneous in the indices. Homogeneity in the orbital indices and invariance under unitary mixing of the orbital states are desirable in a general context and our algebra II has these properties, on par with the usual fermionic or bosonic algebras.

Although algebra I is not invariant under unitary transformations in the orbital or site index k , it is invariant under spin SU(2) transformations. We had already derived the SU(2) algebra (eqs (18) and (19)) for a single site. It is clear that this algebra exists at each site. So, both algebras I and II are invariant under spin rotations.

It is clear that the two algebras are applicable to different physical situations. For applications to condensed matter physics where the lattice site plays a special role (such as the infinite repulsion for electrons at the same site in the Hubbard model), algebra I with the index k representing the lattice site may be relevant. For a more general physical problem where different sets of wave functions related by unitary transformations (for instance position space and momentum space wavefunctions) must be treated in a uniform manner, algebra II may be relevant.

Recent literature on Hubbard model with infinite U contains results which are closer to those expected from algebra I as well as algebra II (See Ruckenstein and Schmitt-Rink 1989 as well as Ogata and Shiba 1990). It appears that the limit of

infinite U does not lead to a unique model and the two algebras provide two possible realizations of the Hubbard model in this limit.

We may also note that algebra II can be easily generalized to the case of an arbitrary number of spin indices n by allowing α , β and γ in eqs (9) and (10) to go over 1 to n . Further study of this generalized algebra will be taken up elsewhere and for the present, we restrict ourselves to the case of $n = 2$.

Hereafter, for the sake of definiteness, we concentrate on algebra II. It is easier to work with, since both the cases of $k = m$ and $k \neq m$ can be treated in a systematic and uniform manner. Results for algebra I can be obtained by combining those of algebra II for equal orbital indices and those of the usual fermionic algebra for different orbital indices. In any case, it is algebra II which has more unfamiliar features (For a further comment on algebra I see §6.3).

3. Calculation of matrix elements

We shall now show how to calculate matrix elements of an arbitrary string of creation and destruction operators in the new algebra II. We assume the existence of a unique vacuum state annihilated by all the annihilators $c_{k\alpha}$

$$c_{k\alpha}|0\rangle = 0. \quad (31)$$

The relations (5)–(8) together with (31) allow the calculation of the vacuum-to-vacuum matrix element of any polynomial in the c 's and c^\dagger 's. To calculate a matrix element which is a monomial in c 's and c^\dagger 's, consider the rightmost c . If it acts on the vacuum to the right, the matrix element vanishes, due to eq. (31). If not, it has one or more c^\dagger immediately to its right. In that case use (6) or (7) to replace cc^\dagger by a zero or a Kronecker δ and $c^\dagger c$. Thus, we have pushed the rightmost c to one step more to the right. Continue this process until c hits $|0\rangle$. Repeat the same for the rightmost c in the remaining matrix elements. It is clear that the process yields zero, unless the number of c 's equals the number of c^\dagger 's in which case the matrix element is a sum of products of Kronecker δ 's. This is similar to the calculation for Fermi operators, except for some important differences described in this and following sections.

The above procedure shows the consistency and completeness of the defining relations (5–8) in the sense that vacuum expectation values of all products of operators can be calculated. In particular, note that one does not need to deal explicitly with the operator products such as $c_{k\sigma}^\dagger c_{m\bar{\sigma}}$ which does not occur in the defining algebra (eqs (5–8)).

Before proceeding further, we find it convenient to introduce a change in notation. The spin up (σ) and spin down ($\bar{\sigma}$) will be denoted by the absence or presence of a bar above the orbital index k :

$$c_k \equiv c_{k\sigma}; \quad c_{\bar{k}} \equiv c_{k\bar{\sigma}}. \quad (32)$$

Consider the matrix element

$$\langle 0 | c_k c_n \cdots c_{\bar{p}} c_q c_r^\dagger c_s^\dagger \cdots c_m^\dagger c_l^\dagger | 0 \rangle$$

where $c_k c_n \cdots c_{\bar{p}} c_q$ is a string of annihilators and $c_r^\dagger c_s^\dagger \cdots c_m^\dagger c_l^\dagger$ is a string of the same number of creators. This matrix element vanishes unless the ordering of spins in the

indices $r\bar{s}\dots ml$ matches exactly with the reverse ordering of spins in the indices $kn\dots\bar{p}q$. For example,

$$\langle 0 | c_k c_n c_{\bar{p}} c_q c_r^\dagger c_s^\dagger c_m^\dagger c_l^\dagger | 0 \rangle \neq 0 \quad (33)$$

but,

$$\langle 0 | c_k c_{\bar{n}} c_{\bar{p}} c_q c_r^\dagger c_s^\dagger c_m^\dagger c_l^\dagger | 0 \rangle = 0. \quad (34)$$

For the spin-matched product of operators, the vacuum matrix element is the antisymmetrized sum of product of Kronecker δ 's in the orbital indices. For example,

$$\langle 0 | c_k c_{\bar{n}} c_m^\dagger c_l^\dagger | 0 \rangle = \delta_{kl} \delta_{nm} - \delta_{km} \delta_{nl}. \quad (35)$$

Thus, in contrast to Fermi operators, the spin labels in some sense decouple from the orbital labels. The value of the matrix element depends only on the orbital labels; however the spin labels do play a crucial role in dictating which of the matrix elements are nonzero, namely only those with exact matching of the spin-order, as defined above.

The above results can be reexpressed in terms of the n -particle Fock-space state vectors defined by:

$$\begin{aligned} |r\bar{s}\dots ml\rangle &= c_r^\dagger c_{\bar{s}}^\dagger \dots c_m^\dagger c_l^\dagger | 0 \rangle \\ \langle lm\dots \bar{s}r| &= \langle 0 | c_l c_m \dots c_{\bar{s}} c_r \end{aligned} \quad (36)$$

We have the results:

- All the state vectors which do not have precisely the same spin order are orthogonal to each other.
- The state $|k\bar{s}\dots mn\rangle$ is antisymmetrical in the orbital labels alone.

$$\text{Examples: } \begin{cases} \langle k\bar{n}pq | q\bar{n}pk \rangle = 0 \\ |k\bar{p}mn\rangle = -|p\bar{k}mn\rangle = |p\bar{k}nm\rangle. \end{cases} \quad (37)$$

$$(38)$$

We see from (38) that, while the space labels can be interchanged by introducing a minus sign for every interchange, the spin labels are frozen. This is a consequence of the relation (24). In fact, the ordering of these frozen spin labels becomes an important characteristic of the state vector. These are the peculiar properties of the particles described by the new algebra II.

Many of the peculiarities of the new algebra II can be traced to the following two equations:

$$\begin{aligned} c_k c_l^\dagger &= 0 \\ c_k c_l^\dagger &= c_{\bar{k}} c_l^\dagger. \end{aligned}$$

Actually the above two are the first and the simplest members of the following infinite sets of null operators and identical operators*.

* In Appendix 2, we shall enlarge the sets of null operators and identical operators further.

Null operators

$$\begin{aligned}
c_k c_l^\dagger &= 0 \\
c_m c_k c_l^\dagger c_n^\dagger &= 0 \\
c_p c_m c_k c_l^\dagger c_n^\dagger c_q^\dagger &= 0, \\
&\vdots
\end{aligned}$$

Identical operators

$$\begin{aligned}
c_l c_k^\dagger &= c_l c_k^\dagger \\
c_l c_k c_m^\dagger c_n^\dagger &= c_l c_k c_m^\dagger c_n^\dagger \\
c_p c_l c_k c_m^\dagger c_n^\dagger c_s^\dagger &= c_p c_l c_k c_m^\dagger c_n^\dagger c_s^\dagger \\
&\vdots
\end{aligned}$$

The above two sets of relations can be summarized by the following two rules for the spin-matching of antinormal products (products of operators with all c 's standing to the left of all c^\dagger 's):

- a) All unmatched antinormal products are zero.
- b) All matched antinormal products are equal.

These rules are closely related to the properties of the vacuum matrix elements already encountered above.

Number operators

Let us define

$$n_k = c_k^\dagger c_k; \quad n_{\bar{k}} = c_{\bar{k}}^\dagger c_{\bar{k}}. \quad (39)$$

It is easy to show that

$$[n_k, c_m] = -\delta_{km} c_m - n_{\bar{k}} c_m \quad (40)$$

$$[n_{\bar{k}}, c_m] = n_{\bar{k}} c_m. \quad (41)$$

These are to be contrasted with the corresponding relations for the usual Fermi operators (distinguished by a \sim)

$$[\tilde{n}_k, \tilde{c}_m] = -\delta_{km} \tilde{c}_m \quad (42)$$

$$[\tilde{n}_{\bar{k}}, \tilde{c}_m] = 0. \quad (43)$$

As a consequence of the extra terms on the right of (40) and (41), n_k and $n_{\bar{k}}$ do not have the usual meaning of number operator. However, the extra terms cancel if we add these two equations and so the total number operator for spin up and down ($n_k + n_{\bar{k}}$) behaves as expected of number operators:

$$[(n_k + n_{\bar{k}}), c_m] = -\delta_{km} c_m. \quad (44)$$

Further, taking a two-particle state $|m\bar{k}\rangle$, one can verify the eigenvalue equations

$$n_k|m\bar{k}\rangle = |m\bar{k}\rangle \quad (45)$$

$$n_{\bar{k}}|m\bar{k}\rangle = 0. \quad (46)$$

Thus, the eigenvalue of n_k is unity while that of $n_{\bar{k}}$ is zero, although the state *appears* to have a particle of label \bar{k} .

These peculiarities of the number operators are related to the decoupling of the space and spin indices and the freezing of the spin-order referred to earlier. Although the label k nominally denotes the orbital state k with spin-up, it has the capacity of manifesting as the spin-down state \bar{k} also. By the same token, c_k and $c_{\bar{k}}$ also should not be associated with unique spin directions. Spin indices get transmuted during interchange of c and c^\dagger .

4. Normal product and Wick expansion

Following the usual practice, we may define normal product as a re-ordering of operators with all c 's standing to the right of all c^\dagger 's, with a negative sign for every interchange of operators. However, because of the peculiar spin-dependence of the algebra II, especially eq. (7), there is a transmutation of spin indices. Hence, consistency requires the presence of more than one term in the definition of the normal product. Thus, we have

$$N(c_m c_n^\dagger) = -(c_n^\dagger c_m + c_n^\dagger c_{\bar{m}}) \quad (47)$$

$$N(c_{\bar{m}} c_n c_k^\dagger) = (c_k^\dagger c_m + c_k^\dagger c_{\bar{m}}) c_{\bar{n}} \quad (48)$$

$$N(c_m c_n^\dagger c_{\bar{k}}) = -(c_n^\dagger c_m + c_n^\dagger c_{\bar{m}}) c_{\bar{k}} \quad (49)$$

$$N(c_m c_n c_k^\dagger c_l^\dagger) = c_k^\dagger c_l^\dagger c_m c_n + c_k^\dagger c_l^\dagger c_{\bar{m}} c_n + c_k^\dagger c_l^\dagger c_m c_{\bar{n}} + c_k^\dagger c_l^\dagger c_{\bar{m}} c_{\bar{n}}. \quad (50)$$

All these can be worked out by using eqs (5–8) and discarding the Kronecker δ 's. If we keep the Kronecker δ 's, then we get the Wick expansion, namely the expansion of any product in terms of normal products. For example,

$$\begin{aligned} c_m c_n c_k^\dagger c_l^\dagger &= \delta_{nk} \delta_{ml} - \delta_{nl} \delta_{mk} - \delta_{nk} (c_l^\dagger c_m + c_l^\dagger c_{\bar{m}}) \\ &\quad + \delta_{mk} (c_l^\dagger c_n + c_l^\dagger c_{\bar{n}}) + \delta_{nl} (c_k^\dagger c_m + c_k^\dagger c_{\bar{m}}) - \delta_{ml} (c_k^\dagger c_n + c_k^\dagger c_{\bar{n}}) \\ &\quad + c_k^\dagger c_l^\dagger c_m c_n + c_k^\dagger c_l^\dagger c_{\bar{m}} c_n + c_k^\dagger c_l^\dagger c_m c_{\bar{n}} + c_k^\dagger c_l^\dagger c_{\bar{m}} c_{\bar{n}}. \end{aligned} \quad (51)$$

On the right hand side we have only normal products. Also, we see explicitly the reincarnation of the opposite spins.

Let us now consider Wick's theorem which is usually stated in the following way: any product of operators $ABCD\dots$ can be expanded into a sum of all possible contractions between pairs of operators with the rest of the operator product replaced by its normal product.

$$ABCD\dots = \underline{AB}\underline{CD} + \dots + \underline{AB}N(CD\dots) + \dots + N(ABCD\dots) \quad (52)$$

where the contraction denoted by the symbol \frown is defined as the vacuum expectation value:

$$\frown AB \equiv \langle 0 | AB | 0 \rangle. \quad (53)$$

Such a theorem is still valid for the new algebra II. A straight-forward application of (52) will yield the expansion of $c_m c_n c_k^\dagger c_l^\dagger$ given in (51). However in the general case, the peculiar spin-behaviour contained in algebra II leads to a modified form of the theorem.

The full statement of the modified form of the Wick's theorem and the complete set of rules for forming the normal product can be worked out for algebra II. These are given in Appendix 2.

5. Factorization

Our results on the calculation of matrix elements with the new algebra suggest the possibility of a factorization of the orbital and spin indices. There are two alternatives which will be considered in this section. In the first, the factors satisfy the usual fermionic and bosonic algebras, but the composite operators do not form a closed algebra. In the second, provided one of the factors satisfy a new algebra, we are able to recover our algebra II.

5.1 Fermion-boson composite

We assume

$$c_{k\alpha} = f_k b_\alpha; \quad \alpha = \sigma, \bar{\sigma} \quad (54)$$

$$[f_k, b_\alpha] = [f_k^\dagger, b_\alpha] = 0 \quad (55)$$

$$\{f_m, f_k^\dagger\} = \delta_{mk}; \quad \{f_m, f_k\} = 0 \quad (56)$$

$$[b_\alpha, b_\beta^\dagger] = \delta_{\alpha\beta}; \quad [b_\alpha, b_\beta] = 0 \quad (57)$$

and ask what is the resulting algebra satisfied by the composite operators $c_{m\alpha}$ and $c_{k\beta}^\dagger$. The answer is given by the following:

$$c_{k\alpha} c_{k\beta} = 0 \quad (58)$$

$$\{c_{k\alpha}, c_{m\beta}\} = 0 \quad (59)$$

$$\{c_{k\alpha}, c_{m\beta}^\dagger\} = \delta_{km} \delta_{\alpha\beta} + \delta_{km} b_\beta^\dagger b_\alpha - f_m^\dagger f_k \delta_{\alpha\beta}. \quad (60)$$

Equations (58) and (59) show that the new exclusion principle and the total antisymmetry of the wave function are automatic consequences. Further, from eq. (60) we note that the usual fermionic anticommutation relation is partially satisfied:

$$\{c_{k\alpha}, c_{m\beta}^\dagger\} = 0 \text{ for } k \neq m \text{ and } \alpha \neq \beta. \quad (61)$$

These are the nice features. However, (60) contains operators other than $c_{m\alpha}$ and $c_{k\beta}^\dagger$ and thus we do not get a closed algebra.

5.2 Factorization of algebra II

In this second alternative, we assume

$$c_{k\alpha} = f_k b_\alpha; \quad \alpha = \sigma, \bar{\sigma} \quad (62)$$

$$[f_k, b_\alpha] = [f_k^\dagger, b_\alpha] = 0 \quad (63)$$

$$\{f_m, f_k^\dagger\} = \delta_{mk}; \quad \{f_m, f_k\} = 0 \quad (64)$$

and then ask what is the algebra satisfied by b_α if we impose the algebra II (eqs (9) and (10)) on $c_{k\alpha}$. The answer is the following:

$$b_\alpha b_\beta^\dagger = \delta_{\alpha\beta} \quad (65)$$

$$\sum_\alpha b_\alpha^\dagger b_\alpha = 1. \quad (66)$$

Thus, factorization ansatz leads to a simple and elegant algebra in the spin indices and the peculiar consequences of algebra II encountered in the earlier sections can be given a more transparent meaning using this factorized algebra.

We may also note that if we define the spin operators (raising, lowering and the diagonal operators) as

$$s_+ = b_\sigma^\dagger b_{\bar{\sigma}} \quad (67)$$

$$s_- = b_{\bar{\sigma}}^\dagger b_\sigma \quad (68)$$

$$s_z = \frac{1}{2}(b_\sigma^\dagger b_\sigma - b_{\bar{\sigma}}^\dagger b_{\bar{\sigma}}); \quad (69)$$

then, the SU(2) algebra (18)–(19) is satisfied as a consequence of (65).

We have already mentioned that algebra II can be generalized to the case of n spin indices. A similar generalization of the factorized algebra can be made by allowing α and β in (65)–(66) to go over 1 to n . Correspondingly, the SU(2) algebra will be replaced by SU(n).

Greenberg (1990) has recently considered a new kind of statistics called *infinite statistics* which involves all the representations of the permutation group and leads to Boltzmann statistics at the quantum level. He shows that the corresponding algebra of the creation and annihilation operators a_α^\dagger and a_β where α and β go over 1 to ∞ , is given by

$$a_\alpha a_\beta^\dagger = \delta_{\alpha\beta}. \quad (70)$$

This is identical to our (65) if we consider the $n \rightarrow \infty$ limit of our algebra. However, our algebra requires (66) in addition. Hence, for infinite number of spin indices, our factorized algebra is equivalent to taking the one-particle sector of the Greenberg system and forming composites of the Greenberg operators with the usual fermionic operators.

In spite of these formal niceties of the factorization ansatz, we must remark that, from a dynamical point of view, the use of the composite operators may be problematic. Our original set of operators $c_{k\alpha}$ are intended to describe physical particles, albeit with strange or unfamiliar properties. What do the factors f_k and b_α describe? There are no physical particles described by these operators in the original system. To ensure

the absence of such particles or excitations described by these "fictitious" operators in the physical spectrum, one may have to impose extra constraints with its attendant problems.

6. Towards physical applications

This paper is mainly concerned with the algebra following from the new exclusion principle; physical applications are outside its scope. However a brief view of some preliminary applications and a comparison with other approaches is offered in this section.

6.1 Partition function and distribution function

Consider the system of free particles obeying the new exclusion principle. Such a system may be described by the Hamiltonian*

$$H = \sum_{i\alpha} \varepsilon_i n_{i\alpha} \quad (71)$$

where $n_{i\alpha}$ is the number operator $c_{i\alpha}^\dagger c_{i\alpha}$ and $c_{i\alpha}$ and $c_{i\alpha}^\dagger$ obey our new algebra. Let us define the partition function Z and the distribution function $\langle n_i \rangle$ (the average number of particles in the orbital state i) in the usual way:

$$Z = \text{Tr} \exp(-\beta H) \quad (72)$$

$$\langle n_i \rangle \equiv \langle n_{i\sigma} + n_{i\bar{\sigma}} \rangle = \frac{1}{Z} \text{Tr}((n_{i\sigma} + n_{i\bar{\sigma}}) \exp(-\beta H)). \quad (73)$$

It is easy to work out Z and $\langle n_i \rangle$ for the "new" fermions (fermions satisfying the new exclusion principle):

$$Z = \prod_i (1 + 2 \exp(-\beta \varepsilon_i)) \quad (74)$$

$$\langle n_i \rangle = 2(2 + \exp \beta \varepsilon_i)^{-1}. \quad (75)$$

These are to be compared with the corresponding expressions for the "old" fermions (fermions satisfying Pauli principle):

$$Z = \prod_i (1 + \exp(-\beta \varepsilon_i))^2 \quad (76)$$

$$\langle n_i \rangle = 2(1 + \exp \beta \varepsilon_i)^{-1}. \quad (77)$$

The above results (74)–(75) are valid for both algebras I and II. In fact the algebra is not used; elementary counting of states is enough.

* Throughout this § 6 as in § 5 we indicate the spin indices σ and $\bar{\sigma}$ explicitly.

6.2 Green's function

We now calculate the single-particle Green's function for the Hamiltonian of (71) where $n_{i\alpha} = c_{i\alpha}^\dagger c_{i\alpha}$ and $c_{i\alpha}, c_{i\alpha}^\dagger$ obey algebra I or II. The Green's function is defined by

$$G_{ii}^\sigma(t) = -i\theta(t)\langle\psi|\{c_{i\sigma}^\dagger(0), c_{i\sigma}(t)\}|\psi\rangle \quad (78)$$

where the time-dependent operators are defined in the Heisenberg picture and $|\psi\rangle$ denotes the ground state of the system. Differentiating with respect to t and using the equation of motion for $c_{i\sigma}(t)$, we get

$$\begin{aligned} i\frac{\partial}{\partial t}G_{ii}^\sigma(t) &= \delta(t)\langle\psi|\{c_{i\sigma}^\dagger(0), c_{i\sigma}(0)\}|\psi\rangle - i\theta(t)\langle\psi|\{c_{i\sigma}^\dagger(0), [c_{i\sigma}(t), H]\}|\psi\rangle \\ &= \delta(t)(1 - \langle n_{i\bar{\sigma}} \rangle) + \varepsilon_i G_{ii}^\sigma(t). \end{aligned} \quad (79)$$

Here we have used the relations

$$\{c_{i\sigma}^\dagger(0), c_{i\sigma}(0)\} = 1 - n_{i\bar{\sigma}} \quad (80)$$

and

$$[c_{i\sigma}(t), (n_{j\sigma}(t) + n_{j\bar{\sigma}}(t))] = \delta_{ij}c_{i\sigma}(t) \quad (81)$$

both of which are valid in algebra I as well as algebra II and we have defined

$$\langle n_{i\bar{\sigma}} \rangle = \langle\psi|n_{i\bar{\sigma}}|\psi\rangle. \quad (82)$$

Equation (79) leads to the following result for the Fourier transform of the Green's function:

$$G_{ii}^\sigma(\omega) = \frac{1 - \langle n_{i\bar{\sigma}} \rangle}{\omega - \varepsilon_i}. \quad (83)$$

We may now compare this result with that following from the conventional approach. For this purpose we consider the Hamiltonian

$$H = \sum_{i\alpha} \varepsilon_i \tilde{n}_{i\alpha} + U \sum_i \tilde{n}_{i\sigma} \tilde{n}_{i\bar{\sigma}} \quad (84)$$

where $\tilde{n}_{i\alpha}$ are the usual number operators $\tilde{c}_{i\alpha}^\dagger \tilde{c}_{i\alpha}$ with the $\tilde{c}_{i\alpha}$ and $\tilde{c}_{i\alpha}^\dagger$ satisfying the *usual* fermionic algebra:

$$\{\tilde{c}_{i\alpha}^\dagger, \tilde{c}_{j\beta}\} = \delta_{ij}\delta_{\alpha\beta} \quad (85)$$

all other anticommutators being zero. We define the Green's function by the same expression as in (78). The Green's function for this model is known to be (Hubbard (1963), Jones and March (1973)):

$$G_{ii}^\sigma(\omega) = \frac{1 - \langle \tilde{n}_{i\bar{\sigma}} \rangle}{\omega - \varepsilon_i} + \frac{\langle \tilde{n}_{i\bar{\sigma}} \rangle}{\omega - \varepsilon_i - U}. \quad (86)$$

Taking the limit $U \rightarrow \infty$ we recover the form of the Green's function obtained with the new algebra (83).

We thus see that the conventional dynamics of infinite repulsion at the same site and our new algebra describing particles without double occupation yield identical results at least in the truncated model considered above. Hence it is hoped that this simplification achieved by the reduction of dynamics to an algebra may lead to a better understanding of the full-fledged Hubbard-model in the limit of infinite U .

6.3 Comparison with Gutzwiller projection and Hubbard algebra

In the literature on the Hubbard model with infinite U , a different approach has been considered (Gutzwiller 1965; and see for instance, Ruckenstein and Schmitt-Rink 1989). To avoid double occupancy at any site, one defines the Gutzwiller projection:

$$g_{i\sigma} \equiv \tilde{c}_{i\sigma}(1 - \tilde{c}_{i\bar{\sigma}}^\dagger \tilde{c}_{i\bar{\sigma}}) \quad (87)$$

where $\tilde{c}_{i\sigma}$ and $\tilde{c}_{i\sigma}^\dagger$ are the usual fermionic operators satisfying the *usual* anticommutation relation (85). It is easy to verify that the Gutzwiller operators satisfy

$$g_{k\sigma} g_{m\bar{\sigma}} + (1 - \delta_{km}) g_{m\bar{\sigma}} g_{k\sigma} = 0 \quad (88)$$

$$g_{k\sigma} g_{m\bar{\sigma}}^\dagger + (1 - \delta_{km}) g_{m\bar{\sigma}}^\dagger g_{k\sigma} = 0 \quad (89)$$

$$g_{k\sigma} g_{m\sigma}^\dagger + g_{m\sigma}^\dagger g_{k\sigma} = \delta_{km} (1 - \tilde{c}_{k\bar{\sigma}}^\dagger \tilde{c}_{k\bar{\sigma}}) \quad (90)$$

$$\{g_{k\sigma}, g_{m\sigma}\} = 0 \quad (91)$$

and all the relations obtained from these by interchanging σ and $\bar{\sigma}$ or by taking hermitian conjugate. On comparing this set of relations with (1)–(4) of algebra I, we see that they are identical except for (90) which involves \tilde{c} and \tilde{c}^\dagger in addition to the Gutzwiller operators. Thus, in contrast to algebra I, the algebra of Gutzwiller operators is not closed.

Let us next define the set of operators $X_i^{\mu\nu}$:

$$\left. \begin{aligned} X_i^{0\sigma} &= c_{i\sigma}; & X_i^{0\bar{\sigma}} &= c_{i\bar{\sigma}} \\ X_i^{\sigma 0} &= c_{i\sigma}^\dagger; & X_i^{\bar{\sigma} 0} &= c_{i\bar{\sigma}}^\dagger \end{aligned} \right\} \quad (92)$$

$$\left. \begin{aligned} X_i^{00} &= c_{i\sigma} c_{i\sigma}^\dagger = c_{i\bar{\sigma}} c_{i\bar{\sigma}}^\dagger \\ X_i^{\sigma\sigma} &= c_{i\sigma}^\dagger c_{i\sigma}; & X_i^{\bar{\sigma}\bar{\sigma}} &= c_{i\bar{\sigma}}^\dagger c_{i\bar{\sigma}} \\ X_i^{\sigma\bar{\sigma}} &= c_{i\sigma}^\dagger c_{i\bar{\sigma}}; & X_i^{\bar{\sigma}\sigma} &= c_{i\bar{\sigma}}^\dagger c_{i\sigma} \end{aligned} \right\} \quad (93)$$

where the c and c^\dagger obey our algebra I. Then, using the algebra I (eqs (1–4)), it is easy to derive the following relations:

$$\sum_\mu X_i^{\mu\mu} = 1 \quad (94)$$

$$X_i^{\mu\nu} X_i^{\lambda\rho} = \delta_{\nu\lambda} X_i^{\mu\rho} \quad (95)$$

$$[X_i^{\mu\nu}, X_j^{\lambda\rho}]_\pm = 0 \text{ for } i \neq j \quad (96)$$

where the Greek indices μ, ν, λ, ρ go over 0, σ and $\bar{\sigma}$ and in the last relation (96), anticommutator (+ sign) is to be used if both the operators are of the fermionic type ($X_i^{0\sigma}, X_i^{0\bar{\sigma}}, X_i^{\sigma 0}$ and $X_i^{\bar{\sigma} 0}$) and commutator (– sign) is to be used otherwise. This set of equations (94)–(96) which may be called Hubbard algebra (Hubbard 1965; Foerster

1989; Ruckenstein and Schmitt-Rink 1989)*, is exactly equivalent to our algebra I. However, the following points must be made.

i) In contrast to our algebra I which contains the irreducible set of relations, the Hubbard algebra includes relations which are derivable from the former. In fact, as we have shown, the new creation and destruction operators c^\dagger and c are the primary operators and all other operators can be consistently expressed in terms of them.

ii) Whereas the single-site relation (95) follows from the identification** (Hubbard 1965)

$$X_i^{\mu\nu} = |i\mu\rangle\langle i\nu|, \quad (97)$$

the multi-site ($i \neq j$) relation (96) does not follow. If one uses the Gutzwiller-projection in terms of usual fermionic operators (Ruckenstein and Schmitt-Rink 1989):

$$X_i^{0\sigma} = g_{i\sigma} = \tilde{c}_{i\sigma}(1 - \tilde{n}_{i\sigma}), \quad (98)$$

the multisite relation (96) can be obtained, but then some of the single-site relations will be altered, as shown in (90) above. So, in the literature, an ambiguous attitude towards the derivation of Hubbard algebra seems to have been adopted. Actually, the multisite relation *cannot* be derived, *without further assumptions*. With suitable assumptions, which were already mentioned in §2, one can get either algebra I or II.

Thus, our procedure of expressing everything in terms of new c and c^\dagger obeying new algebras provides a unified framework which facilitates comparison between various approaches.

7. Summary and discussion

We have found the algebra for fermions obeying a new exclusion principle for spin which forbids the occupation of more than a single particle in any orbital state. Many of the peculiarities following from this algebra have been elucidated through the calculation of typical matrix elements as well as through the normal order operation and the Wick expansion of operator products. Factorized version of the algebra also has been discussed. Some preliminary applications have been indicated.

It may be useful to compare the statistics corresponding to the new algebra II with the well-known parastatistics (Green 1953; Greenberg and Messiah 1964). In para-fermistics of order n , at most n para fermions can occupy the same state. In contrast, for the algebra II given by (9)–(10) with α, β going over 1 to n , at most one fermion occupies the set of n states all having the same (orbital) index. To emphasize this contrast with parastatistics, one may call the new statistics implied by algebra II as *orthostatistics* and the new particles as *orthofermions*.

We must stress that algebra II leads to antisymmetry of the wavefunction in the orbital indices alone (just as for spinless fermions). By superposition of the states

*In some of these references, the algebra is stated in a form which is either incomplete or ambiguous. Specifically, note that from eq. (95) both commutation *and* anticommutation relations can be derived for all pairs of X operators at a single site, be they of fermionic or bosonic type.

** Hubbard's definition of $X_i^{\mu\nu}$ (eq. (97)) should be really understood as an appropriate direct product of $|i\mu\rangle\langle i\nu|$ at site i and (local) identity operators at all other sites.

with different spin-ordering, states symmetric in spin and hence totally antisymmetric (in space and spin) can be constructed. But, the point is that this does not follow from the algebra itself, in contrast to the case of the usual fermionic algebra from which total antisymmetry follows. For algebra II, total antisymmetry has to be imposed as an extra condition, if required.

In this context, one may naturally raise the question whether an algebra with the following properties exists. It must incorporate the new exclusion principle, it must be invariant under unitary transformations in the orbital indices, total antisymmetry in the orbital and spin indices must follow from the algebra and it must be a closed algebra involving only c and c^\dagger . The answer to this question appears to be negative and the result can possibly be proved. This, as well as the construction of a new algebra which achieves total antisymmetry at the cost of involving a certain new class of operators will be reported in a later publication.

Following are some interesting extensions, generalizations and applications:

- (a) Construction of a relativistic quantum field theory based on the algebra II.
- (b) A detailed study of the algebra II for arbitrary number n of spin indices and specially for $n \rightarrow \infty$.
- (c) Extension of Grassmann calculus to incorporate the new exclusion principle.
- (d) Symmetric or bosonic version of the algebras I and II.
- (e) Possible connections between the algebra II on the one hand and other mathematical constructs such as supersymmetry algebra, braid group and braid statistics on the other hand.
- (f) Physical applications of the new algebras to problems of condensed matter physics.

These may be taken up in the future.

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Appendix 1. Representation of the single-site operators

For the case of the single site, the complete orthonormal set of kets is $|0\rangle$, $|\sigma\rangle$ and $|\bar{\sigma}\rangle$ which are the no-particle state, the spin-up particle state and the spin-down particle state respectively. Thus it is easy to see that

$$c_\sigma = |0\rangle\langle\sigma|, \quad c_\sigma^\dagger = |\sigma\rangle\langle 0|, \quad (A1)$$

$$c_{\bar{\sigma}} = |0\rangle\langle\bar{\sigma}|, \quad c_{\bar{\sigma}}^\dagger = |\bar{\sigma}\rangle\langle 0|. \quad (A2)$$

The completeness relation is

$$|0\rangle\langle 0| + |\sigma\rangle\langle\sigma| + |\bar{\sigma}\rangle\langle\bar{\sigma}| = 1. \quad (A3)$$

Using these equations and the orthonormality relations, our algebra (11)–(14) can be derived.

If we choose the basis vectors:

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\sigma\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |\bar{\sigma}\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad (\text{A4})$$

we get the matrix representations:

$$c_\sigma = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad c_\sigma^\dagger = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (\text{A5})$$

$$c_{\bar{\sigma}} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad c_{\bar{\sigma}}^\dagger = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}. \quad (\text{A6})$$

The above is to be contrasted with the case of the usual spin $\frac{1}{2}$ fermions for which the vector space is 4-dimensional and is a direct product: $\{|0\rangle, |\sigma\rangle\} \otimes \{|0\rangle, |\bar{\sigma}\rangle\}$. It is well-known that the creation and destruction operators for this usual case can be built out of the $SU(2) \otimes SU(2)$ generators in the fundamental representation $\tau_i \otimes \tau_j$ where τ_i are the Pauli matrices (one $SU(2)$ for spin up and the other for spin down). In contrast, the operators in (A5)–(A6) are constructed out of the $SU(3)$ generators in the fundamental representation $\mathbf{3}$. Explicitly,

$$c_\sigma = \frac{1}{2}(\lambda_1 + i\lambda_2), \quad c_\sigma^\dagger = \frac{1}{2}(\lambda_1 - i\lambda_2) \quad (\text{A7})$$

$$c_{\bar{\sigma}} = \frac{1}{2}(\lambda_4 + i\lambda_5), \quad c_{\bar{\sigma}}^\dagger = \frac{1}{2}(\lambda_4 - i\lambda_5) \quad (\text{A8})$$

where the λ_i are the Gell-Mann matrices of $SU(3)$.

When the orbital or site label $k = 1 \dots m$ is included, the operators $c_{k\sigma}$ and $c_{k\bar{\sigma}}$ can be written as $3^m \times 3^m$ matrices, which are generators of $SU(3^m)$. Thus, these new operators are represented by odd-dimensional matrices in contrast to the usual fermionic creation and destruction operators which are represented by even-dimensional ($4^m \times 4^m$) matrices of $SU(2^m) \otimes SU(2^m)$.

Appendix 2. Rules for normal product and Wick expansion

The rules for writing down the normal product and the Wick expansion for an arbitrary operator product that follow from our algebra II are given here. These may prove useful for calculations in any dynamical theory based on the new algebra.

Normal product

Step 1: From the given operator product expression, form all compact antinormal pairs.

Compact antinormal pair (CAP) is defined to be an antinormal pair between a c_m and a c_n^\dagger such that no unpaired c or c^\dagger appears between c_m and c_n^\dagger . We shall denote CAP by the symbol \smile . The compact antinormal pairing of all possible operators in a given operator product is unique.

Examples:

$$\begin{aligned} & c_m c_n c_k^\dagger, \quad c_m c_n c_k^\dagger c_l^\dagger, \\ & c_s c_t c_k c_l c_m c_n c_p c_q c_r^\dagger. \end{aligned}$$

Note that $c_m c_n c_k^\dagger$ and $c_m c_n c_k^\dagger c_l^\dagger$ are not CAP.

Step 2: If the spins on the c and c^\dagger appearing in any of the CAP are not matched, the given operator product vanishes and so does its normal product.

Examples:

$$\begin{aligned} & c_k c_l c_m c_n c_p^\dagger c_q^\dagger = 0 \\ & c_k c_l c_m c_n c_p c_q c_r^\dagger c_s^\dagger c_t^\dagger c_u^\dagger c_v c_w = 0 \end{aligned} \quad (A9)$$

$$c_k c_l c_m c_n c_p c_q c_r^\dagger c_s^\dagger c_t^\dagger c_u^\dagger \dots = 0. \quad (A10)$$

Note that this step enlarges the set of null operators introduced in §3, to operators that are not in antinormal order. Operators with spin-unmatched CAP's are null.

Step 3: In case the spins in each CAP match, find out the rank of the operator product, the rank being defined as the total number of the CAP links. If the rank is m , write the 2^m terms of the normal product, each with a different matched spin-order as shown in the example below.

If no unpaired c or c^\dagger remains, multiply the result by $(-1)^P$ where P is the number of interchanges of the various operators. This is the complete answer.

Example:

$$N(c_k c_l c_p c_q^\dagger) = -(c_l^\dagger c_q^\dagger c_k c_p + c_l^\dagger c_q^\dagger c_k c_p + c_l^\dagger c_q^\dagger c_k c_p + c_l^\dagger c_q^\dagger c_k c_p). \quad (A11)$$

Since $m = 2$, the number of spin-transmuted terms on the right is four.

Step 4: If there remain unpaired c or c^\dagger after the formation of all CAP's, shift all such unpaired c or c^\dagger to the extreme right or left respectively with their spins intact. For the rest, use step 3. Finally multiply the answer by $(-1)^P$.

Examples:

$$N(c_m c_n c_k c_l^\dagger) = N(c_k c_l^\dagger) c_m c_n \quad (A12)$$

$$N(c_m c_n c_k^\dagger c_l^\dagger c_p c_q) = c_m^\dagger N(c_n c_k^\dagger c_l^\dagger c_p c_q) \quad (A13)$$

$$N(c_m c_n c_k^\dagger c_l^\dagger c_p c_q) = c_k^\dagger N(c_m c_n c_p c_q) \quad (A14)$$

The N product occurring on the right side can be evaluated using step 3. The point of the step 4 is that there is no spin transmutation for the operators not linked by CAP.

Wick expansion

Step 1: Form all the compact antinormal pairs (CAP) already defined. Let us assume that all of them are spin-matched, otherwise the whole expression is zero. If there remain unpaired c or c^\dagger note their spins as well as the order in which they occur.

Step 2: Write the usual Wick expansion with all possible contractions, *even including* contractions between spin-unmatched c and c^\dagger . Assign the following values for the contractions:

$$\underline{c_k c_m^\dagger} = \underline{c_{\bar{k}} c_{\bar{m}}^\dagger} = \underline{c_{\bar{k}} c_m^\dagger} = \underline{c_k c_{\bar{m}}^\dagger} = \delta_{km}. \quad (\text{A15})$$

All other contractions are zero.

Step 3: The uncontracted operators are to be left in the normal ordered form. However, this normal ordering is, in general, different from the normal product defined through the rules given earlier in this appendix. Spin-transmutation must be used for all the pairs except for the unpaired operators identified in step 1. We shall distinguish this normal ordering by the symbol M .

Step 4: Rewrite the spins of the unpaired c or c^\dagger such that it corresponds to the spin-ordering noted in step 1. Every term must have the sign $(-1)^P$. This is the complete answer.

Examples:

$$\text{a) } c_{\bar{k}} c_l c_m c_n^\dagger = M(c_{\bar{k}} c_l c_m c_n^\dagger) + M(c_{\bar{k}} c_l c_m c_n^\dagger) + M(c_{\bar{k}} c_l c_m c_n^\dagger) + N(c_{\bar{k}} c_l c_m c_n^\dagger) \quad (\text{A16})$$

$$= \delta_{mn} c_{\bar{k}} c_l - \delta_{ln} c_{\bar{k}} c_m + \delta_{kn} c_l c_m - (c_n^\dagger c_m + c_n^\dagger c_{\bar{m}}) c_{\bar{k}} c_l. \quad (\text{A17})$$

The unpaired operators in the given expression are $c_{\bar{k}} c_l$ and these dictate the spin-order of c c occurring in each term of the Wick expansion.

$$\begin{aligned} \text{b) } c_k c_l^\dagger c_{\bar{m}} c_n c_p c_q^\dagger &= M(c_k c_l^\dagger c_{\bar{m}} c_n c_p c_q^\dagger) + M(c_k c_l^\dagger c_{\bar{m}} c_n c_p c_q^\dagger) \\ &+ M(c_k c_l^\dagger c_{\bar{m}} c_n c_p c_q^\dagger) + M(c_k c_l^\dagger c_{\bar{m}} c_n c_p c_q^\dagger) + M(c_k c_l^\dagger c_{\bar{m}} c_n c_p c_q^\dagger) \\ &+ M(c_k c_l^\dagger c_{\bar{m}} c_n c_p c_q^\dagger) + M(c_k c_l^\dagger c_{\bar{m}} c_n c_p c_q^\dagger) \\ &+ M(c_k c_l^\dagger c_{\bar{m}} c_n c_p c_q^\dagger) + N(c_k c_l^\dagger c_{\bar{m}} c_n c_p c_q^\dagger). \end{aligned} \quad (\text{A18})$$

$$\begin{aligned} &= \delta_{kl} \delta_{pq} c_{\bar{m}} c_n - \delta_{kl} \delta_{nq} c_{\bar{m}} c_p + \delta_{kl} \delta_{mq} c_{\bar{n}} c_p \\ &+ \delta_{kq} (c_l^\dagger c_m + c_l^\dagger c_{\bar{m}}) c_{\bar{n}} c_p - \delta_{kl} (c_q^\dagger c_p + c_q^\dagger c_{\bar{p}}) c_{\bar{m}} c_n \\ &- \delta_{pq} (c_l^\dagger c_k + c_l^\dagger c_{\bar{k}}) c_{\bar{m}} c_n + \delta_{nq} (c_l^\dagger c_k + c_l^\dagger c_{\bar{k}}) c_{\bar{m}} c_p \\ &- \delta_{mq} (c_l^\dagger c_k + c_l^\dagger c_{\bar{k}}) c_{\bar{n}} c_p + N(c_k c_l^\dagger c_{\bar{m}} c_n c_p c_q^\dagger). \end{aligned} \quad (\text{A19})$$

In particular, it must be pointed out that

$$M(c_k c_l^\dagger c_{\bar{m}} c_n c_p c_q^\dagger) \neq \delta_{kq} N(c_l^\dagger c_{\bar{m}} c_n c_p). \quad (\text{A20})$$

According to our earlier rules on N product, there is no spin-transmutation in $N(c_l^\dagger c_{\bar{m}} c_n c_p)$ since there is no CAP in this N product:

$$N(c_l^\dagger c_{\bar{m}} c_n c_p) = c_l^\dagger c_{\bar{m}} c_n c_p. \quad (\text{A21})$$

But, spin-transmutation does occur in the M product for one pair as specified in step 3 of the Wick expansion and hence

$$M(c_k c_l^\dagger c_{\bar{m}} c_n c_p c_q^\dagger) = \delta_{kq} (c_l^\dagger c_m + c_l^\dagger c_{\bar{m}}) c_{\bar{n}} c_p. \quad (\text{A22})$$

Finally, we note that, as a consequence of these rules for the Wick expansion and the normal product, the set of identical operators introduced in § 3 gets enlarged. All the operator products differing only in their spin-order are identical to each other, provided they contain no unpaired operators after all the CAP links are formed. For example,

$$\underbrace{c_m c_n c_k^\dagger c_l c_p^\dagger c_q^\dagger}_{\text{CAP links}} = \underbrace{c_m c_n c_k^\dagger c_l c_p^\dagger c_q^\dagger}_{\text{CAP links}} \quad (\text{A23})$$

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