Composite particles in nonrelativistic many-body theory: Foundations and statistical mechanics

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A new fundamental theory of composite particles in nonrelativistic many-body systems is developed. The theory is constructed making use solely of the physical Fock space for the basic elementary particles which comprise the many-body system. In this manner exchange symmetry in the elementary particles is exact. Physical composite particle creation and annihilation operators are introduced and these operators satisfy exact Bose (Fermi) commutation (anticommutation) relations depending on whether the composites correspond to bosons or to fermions. Commuting physical occupation number operators for composite particles are then constructed in the usual manner from the composite creation and annihilation operators. These number operators are highly dressed in terms of the basic elementary particle operators. Finally, the foundations of statistical mechanics for bound composite particles are formulated in terms of the appropriate occupation number operators.

I. INTRODUCTION

Nonrelativistic many-body theory describes systems made up of interacting elementary particles for which the interaction is presumed known. Further, the total number of elementary particles of each type usually is taken to be conserved. It is generally believed that all observables can be described in terms of quantities constructed from coordinates, spin, etc., of the elementary particles which make up the system. It is assumed that the time evolution of the state is determined by the nonrelativistic quantummechanical Hamiltonian for the full system. The Hamiltonian also may contain contributions from external fields. In the language of second quantization, every observable may be represented by an operator, which in turn may be expressed in terms of creation and annihilation operators for the elementary particles. We assume that this quantum-mechanical description is complete.

On the other hand, there are remarkably accurate descriptions of complex systems given in terms of interacting composite particles. Not only for very tenuous systems, but also for fairly dense systems, one finds accurate accounts of composite particle reactions, equilibria, and kinetic effects such as diffusion all expressed in terms of composite molecular dynamics. The relative stability of nuclei, atoms, and molecules when kinetic energies are not too large is, of course, the main reason why the composites maintain or nearly maintain their identities even during these interactions.

The Ehrenfest-Oppenheimer¹ theorem states

that composites made up of odd numbers of Fermi-Dirac-type elementary particles (fermions) behave nearly as fermion composites, and composites made up of even numbers of elementary fermions behave nearly as Bose-Einstein composites (bosons). In either case the composites may have any number of elementary bosons. That is, if the total fermion number F is odd the composites are approximately fermions, and if F is even the composites are approximately bosons. Nearly or approximately here means that if spatial separations are large or if composite interactions are small, one finds the designated composite exchange symmetry to be satisfied. Any fundamental theory of composite particles must take into account the exact exchange symmetry as reflected by that of the basic elementary particles.

There are three basic problems, each of singular importance, in a first-principles approach to composite particles in many-body systems. The first has to do with the description of a single composite embedded in a many-body sea. It is clear that an "atom" in a dense plasma may be something quite distinct from an isolated atom. The type of considerations required for a solution to this problem lies somewhat outside the realm of what is common in physical theory. An interesting account of this problem is provided by Golden in his book² on chemical kinetics. Golden states "It is now evident that a central problem in the construction of a mathematical theory of chemical behavior may be identified with the question, 'What is meant by a molecule?'."

There are various approaches to this problem. For example, one could try to find eigenvectors

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of reduced density operators, and then use these to describe individual composites. Or, one could try to construct individual composite wave functions by building up the total wave function for the system in terms of them and then using a variational principal for the energy to determine the "best" such composite. Green's-function approaches may also be used.

The main results of this paper deal not with the first problem but with the second. We assume that the first problem has been solved (no easy task) and that we have at our disposal a satisfactory description of what is meant by individual composites in the particular many-body context of interest. The problem then is how to formulate a description of the given many-body system in terms of many composites interacting with each other. (They may, of course, also interact with elementary particles.)

This problem has received a good deal of attention starting with the works of Wentzel,³ Dyson,⁴ and, in particular, Girardeau.⁵ Girardeau has systematized the idea that composites can be treated as ideal composite fermions or bosons in an ideal state space. However, the ideal state space is too large, so subsidiary conditions must be imposed on the ideal state vectors if they are to correspond to physical many-body states. This means that simple ideal space expressions such as ideal composite number operators have no simple interpretation beyond first approximation in the physical state space.

The present theory operates entirely in the physical Hilbert space of the many-body system. All operators are constructed from the elementary particle creation and annihilation operators. Thus all exchange effects are automatically taken into account and there is no problem dealing with unphysical states. We establish the existence of well-defined operators from which observables dealing with composites may be constructed. The use of these operators then facilitates the establishment of the foundations of statistical mechanics for composite particles in a many-body setting.

The third problem is that of practical computation starting with the basic formalism developed here. The mathematical structure of the theory is not conceptually difficult, but it requires somewhat different techniques from the ones we are used to, so that new types of perturbation expressions, etc., are required. The difficulties associated with practical computation cannot be minimized but should not be regarded too negatively either. We recall the long periods of time elapsed between the establishment of many basic equations and discovery of systematic and practical solutions.

II. SIMPLE COMPOSITE SYSTEMS

We consider a many-body system which contains a large number of elementary particles (e.g., various nuclei and electrons). The elementary particles interact through a given nonrelativistic Hamiltonian 3C. Depending upon the state of the system, some of the elementary particles (or even all of them) may combine to form bound composite particles. That is, bound ions, atoms, or molecules may for under suitable physical conditions.

A system which is readily describable in terms of a single composite species is called a *simple* composite system. As an example, ordinary helium gas may be considered to be a simple system, that is, a collection of interacting helium atoms, although from a more fundamental point of view it is a many-body system consisting of helium nuclei and electrons.

We wish to find a suitable description of such interacting composite systems starting with the basic properties of the interacting elementary particles. We assume that we know how to describe a single composite structure in terms of its elementary particle constituents. That is, we assume that the first main problem discussed in the Introduction has been satisfactorily solved. The solution of this part of the problem can be given in the form of a set $\{\psi_{\alpha}\}_{\alpha=1}^{\alpha_0}$ of wave functions ψ_{α} which define the bound states of the composite particle. The label α refers to the internal degrees of freedom and also to the center-of-mass degrees of freedom. The wave functions ψ_{α} may be, and in general will be, quite different from the wave functions of an isolated composite. As far as our development here is concerned, we assume that the ψ_{α} are orthonormal, $\langle \psi_{\alpha} | \psi_{\alpha'} \rangle \equiv \langle \alpha | \alpha' \rangle$ $=\delta(\alpha, \alpha')$, but that they form an incomplete set of vectors in the state space of the elementary particles making up the composite. Symbolically, $\sum_{\alpha} |\alpha\rangle\langle\alpha|$ is a projection operator which is less than unity.

We use the formalism of second quantization and designate by \mathfrak{F} the Fock space corresponding to the elementary particles. Let $a(i), b(j), \ldots$; $a(i)^*, b(j)^*, \ldots$, be annihilation and creation operators for the elementary particles of types a, b, \ldots , where i, j, \ldots , label complete orthónormal single particle states. Then \mathfrak{F} is spanned by the complete orthonormal set of vectors

$$\{ \{ n_{a}(i) \}, \{ n_{b}(j) \}, \dots \}$$

$$= \prod_{i, j, \dots} \frac{[a(i)^{*}]^{n(i)} [b(j)^{*}]^{n(j)}}{\sqrt{n(i)!} \sqrt{n(j)!}}, \dots | 0 \rangle$$

$$= | n_{a}, n_{b}, \dots \rangle \equiv | n \rangle,$$

$$(2.2)$$

where $n_a = \{n_a(i)\}_{i=1}^{\infty}$ stands for the set of occupation numbers $n_a(i)$ (=0, 1, 2, ...) of the elementary particle of type *a*. The vacuum state is $|0\rangle$ and it is understood that in Eq. (2.1) the product is ordered,

$$\frac{[a(1)^*]^{n(1)}}{\sqrt{n(1)!}} \frac{[a(2)^*]^{n(2)}}{\sqrt{n(2)!}} \dots |0\rangle$$

We may assume that $\sum_{i=1}^{\infty} n(i) < \infty$ for each type of elementary particle, so we deal with many body systems having arbitrarily large, but finite, numbers of elementary particles. The vectors given by Eq. (2.1) are orthonormal,

$$\langle n_a, n_b, \dots | n'_a, n'_b, \dots \rangle \equiv \langle n | n' \rangle$$

= $\delta(n_a, n_b, \dots; n'_a, n'_b, \dots)$
= $\delta(n; n'),$

and complete,

$$\sum_{n} |n\rangle \langle n| = 1_{\mathfrak{F}}.$$
 (2.3)

By $1_{\mathfrak{F}}$ is meant the unit operator on \mathfrak{F} and the sum in Eq. (2.3) is understood as a strong operator limit.

A single composite A having the wave function ψ_{α} is represented in F by

$$|\alpha\rangle = A^*_{(\alpha)}|0\rangle, \qquad (2.4)$$

where $\psi_{\alpha}(I) = \langle I | \alpha \rangle$, and where I is a suitable set of coordinates and spins for the elementary particles making up the composite. (See Appendix A.) The single composite creation operator A^* is expressed linearly in terms of products of the elementary particle creation operators $a(i)^*, b(j)^*, \ldots^6$ For example, a single bound hydrogen atom can be represented by the vector

$$|\alpha\rangle = \sum_{i,j} a(i) * b(j) * \langle ij | \alpha \rangle | 0 \rangle, \qquad (2.5)$$

where $\langle ij | \alpha \rangle = \psi_{\alpha}(ij)$ is the wave function for the given bound state $|\alpha\rangle$, $a(i)^*$ is the creation operator for the proton in the single proton state $|i\rangle$, and $b(j)^*$ is that of the electron in the single electron state $|j\rangle$.

The composite state vectors $|\alpha\rangle$ are taken to be orthornormal,

$$\langle \alpha | \alpha' \rangle = \delta(\alpha, \alpha'),$$

but, in general, incomplete in the single composite particle subspace of \mathfrak{F} . That is,

$$\sum_{\alpha} |\alpha\rangle \langle \alpha | = \hat{B}_A \tag{2.6}$$

is an orthogonal projection operator (*projector*) on the single bound composite particle subspace of $\mathfrak{F}: \hat{B}_A^2 = \hat{B}_A = \hat{B}_A^*$, and, in general, $\hat{B}_A < \hat{P}_A$, where \hat{P}_A is the projector on the full single composite particle subspace of \mathcal{F} . Physically this means, in general, that ionized states (scattering states, etc.) of A are not included in the bound states $|\alpha\rangle$. Ions will not be excluded in the general theory but will be treated as different composite particles.

The composites A will be called boson composites if the number of elementary fermions making up A is even (including zero) and will be called fermion composites if their fermion number is odd. The composite annihilation operators $A(\alpha)$ = $[A(\alpha)^*]^*$ and creation operators $A(\alpha)^*$ do not satisfy simple commutation or anticommutation relations.⁶ However, on the vacuum state

 $[A(\alpha), A(\alpha')^*]_{\pm}|0\rangle = \delta(\alpha, \alpha')|0\rangle,$

where the plus sign (anticommutator) holds for fermion composites, and the minus sign (commutator) holds for boson composites.

If the composite particle annihilation and creation operators satisfied elementary commutation (anticommutation) relations, then the vectors

$$|N_{A}\rangle \equiv |\{N(\alpha)\}\rangle \equiv \prod_{\alpha} \frac{[A(\alpha)^{*}]^{N(\alpha)}}{\sqrt{N(\alpha)!}} |0\rangle$$
(2.7)

would be orthonormal and *would* correspond to physical states in which there are $N(\alpha)$ composites of type A in the single composite particle state $|\alpha\rangle$. We note that for fermion composites $N(\alpha) = 0, 1$, since for $N(\alpha) \ge 2$, $[A(\alpha)^*]^{N(\alpha)} = 0$. We consider now the vectors

$$|N_A, n\rangle \equiv \prod_{\alpha} \frac{[A(\alpha)^*]^{N(\alpha)}}{\sqrt{N(\alpha)!}} |n\rangle, \qquad (2.8)$$

where $N(\alpha) = 0, 1, 2, ...$, and $|n\rangle$ are the vectors defined by Eq. (2.2). The vectors $|N_A, n\rangle$ are not orthonormal for $N_A \neq 0$ and are overcomplete in \mathfrak{F} since $\{|0,n\rangle\}$ is an orthonormal complete set in \mathfrak{F} .

If, however, we restrict the elementary particle states by introducing large but finite cutoffs i_0, j_0, \ldots for the elementary particle states so that $1 \le i \le i_0, 1 \le j \le j_0, \ldots, 1 \le \alpha \le \alpha_0$, then we may expect for suitable values $i_0, j_0, \ldots, \alpha_0$ that, with certain mild technical assumptions concerning the nature of the single composite particle states $|\alpha\rangle$, the vectors $|N_A, n\rangle$ will be linearly independent. Let us introduce the notation

$$\{|N_A, n_c\rangle\} = \{|N_A, n\rangle\}_{i \le i_0, j \le j_0, \dots}.$$
(2.9)

Then we may take the set $\{|N_A, n_c\rangle\}$ to be linearly independent. In Appendix A we outline arguments for the validity of the above statements. On the other hand, in general, the vectors $|N_A, n_c\rangle$ are not complete (total) in \mathfrak{F} . We do argue that we may choose $i_0, j_0, \ldots, \alpha_0$ and the set $\{\psi_c\}_{\alpha=1}^{\alpha_0}$, $\alpha_0 < \infty$, in such a way that the vectors $|N_A, n_c\rangle$ span a subspace P_c of \mathfrak{F} which is sufficiently large to be comsidered the space of states for all nonrelativistic many-body states of interest and at the same time the $|N_A, n_c\rangle$ are linearly independent. The main technical assumption concerning the states $|\alpha\rangle$ is that they have *no* cutoff in the elementary particle states $|i\rangle$, $|j\rangle$,..., from which they are constructed.

We may orthogonalize the collection $\{|N_A, n_c\rangle\}$ by the procedure, originally found by des Cloizeaux⁷ and used by the present authors and Girardeau to construct completely orthogonalized plane waves.⁸ (Reference 8 will be referred to simply as SBG.)

The orthogonal vectors which would result from the orthogonalization of the set $\{|N_A, n_c\rangle\}$ have the property⁹ that they are as close as possible (in the sense that the sum of the squares of the norms of the difference between vectors in the original set and the corresponding orthonormal vectors is a minimum) to the original set of nonorthogonalized vectors. The presence of products of many elementary particle creation operators in $|N_A, n_c\rangle$ means that these vectors (when normalized) represent states which can be considered to possess various bound composites corresponding to the $N(\alpha)$, but the elementary particle part n_c cannot be close to representing free or unbound elementary particles. In fact, for fixed $\{N(\alpha)\}$, linear combinations of $|N_A, n_c\rangle$ can be made to closely approximate states having more than N_A composite particles. Since we wish to construct states corresponding to definite numbers of bound composites, we must seek a more representative basis for our construction than $\{|N_A, n_c\rangle\}$. This is achieved through the use of vectors which are orthogonal to all vectors having one or more composites. Such vectors may be thought of as corresponding to completely ionized or free states of the elementary particles. Girardeau has termed such vectors completely orthogonal (to all bound states) vectors. We now determine how to construct these completely orthogonal vectors.

We denote by $|f\rangle$ any completely orthogonal vector. This vector must be orthogonal to every vector $|N_A, n_c\rangle$ for which $N_A \neq 0$ [i.e., some $N(\alpha)$ must be nonzero]. Thus

$$\langle f | N_A, n_c \rangle = 0, \quad N_A \neq 0$$
 (2.10)

and we observe that

$$A(\alpha)|f\rangle = 0 \forall \alpha$$
 (2.11)

is a necessary and sufficient condition that $|f\rangle$ be completely orthogonal to the bound states. If \hat{P}_{B} is the projector on the subspace P_{B} of F corresponding to vectors having one or more bound composites, we may express the conditions Eq. (2.10) and Eq. (2.11) by

$$\hat{b}_{B}^{1}|f\rangle = |f\rangle, \qquad (2.12)$$

where $\hat{P}_{B}^{i} = 1_{\mathcal{F}} - \hat{P}_{B}$ is the projector on the orthogonal subspace P_{B}^{i} orthogonal to P_{B} . The projector \hat{P}_{B} is constructed by first forming the positive operator

$$\hat{g}_{B} \equiv \sum_{N_{A} \neq 0} |N_{A}, n_{c}\rangle \langle N_{A}, n_{c}|, \qquad (2.13)$$

and observing that

$$\hat{g}_{\boldsymbol{B}}|f\rangle = 0, \qquad (2.14)$$

since $|f\rangle$ is orthogonal to each $|N_A, n_c\rangle$, $N_A \neq 0$. On the other hand, if $|g\rangle$ is orthogonal to $|f\rangle$, $\langle f|g\rangle = 0$,

$$\lim_{\mathbf{g}\to 0} (\hat{g}_{\mathbf{B}} + \mathcal{E}\mathbf{1}_{\mathbf{g}})^{-1} \hat{g}_{\mathbf{B}} |g\rangle = |g\rangle.$$
(2.15)

Therefore, as discussed in SBG (appendix), we may write

$$\hat{P}_{B} = s - \lim_{\delta \to 0} (\hat{g}_{B} + \delta \mathbf{1}_{\mathfrak{F}})^{-1} \hat{g}_{B}$$
(2.16)

$$= s - \lim_{\boldsymbol{\delta} \to 0} \hat{g}_{\boldsymbol{B}} (\hat{g}_{\boldsymbol{B}} + \mathcal{E} \mathbf{l}_{\boldsymbol{\mathfrak{F}}})^{-1}, \qquad (2.17)$$

where $s - \lim$ (strong operator limit) means that for $|\psi\rangle$ in the domain of \hat{g}_{R} ,

$$\hat{P}_{B}|\psi\rangle = \lim_{\delta \to 0} \left(\hat{g}_{B} + \delta \mathbf{1}_{\mathfrak{F}}\right)^{-1} \hat{g}_{B}|\psi\rangle.$$
(2.18)

Since \hat{P}_B is a bounded operator it may be defined (by continuity) on the entire Hilbert space \mathfrak{F} . We have found other useful forms for \hat{P}_B , \hat{P}_B^{\perp} , e.g.,

$$\hat{P}_{B}^{\perp} = s - \lim_{\lambda \to \infty} \exp(-\lambda \hat{g}_{B}), \qquad (2.19)$$

which can be established directly.

We now introduce vectors $|N_A, n_c, f\rangle$ which more nearly than $|N_A, n_c\rangle$ correspond to states having N_A composite particles and n_c free or unbound elementary particles:

$$|N_{A}, n_{c}, f\rangle \equiv \prod_{\alpha} \frac{[A(\alpha)^{*}]^{N(\alpha)}}{\sqrt{N(\alpha)!}} \hat{P}_{B}^{1}|n_{c}\rangle. \qquad (2.20)$$

The vectors $|N_A, n_c, f\rangle$ are also linearly independent (see Appendix C).

The orthonormalization of the vectors $|N_A, n, f\rangle$ is accomplished by the procedure given in SBG (appendix). Let \hat{g} be defined by

$$\hat{g} \equiv \sum |N_{A}, n_{c}, f\rangle \langle N_{A}, n_{c}, f|, \qquad (2.21)$$

where the sum is taken over all $N(\alpha)$, n(i), n(j),... and is understood to be the strong limit as each N,n goes to infinity. The operator $\hat{g}_{g} \equiv 1_{g} \mathcal{E} + \hat{g}$ is strictly positive for $\mathcal{E} > 0$ and is used to form the orthonormal set $\{|N_{A}, n_{c}, f\rangle^{\sim}\}$ of vectors $|N_{A}, n_{c}, f\rangle^{\sim}$ by means of the prescription

$$|N_{\boldsymbol{A}}, \boldsymbol{n}_{c}, \boldsymbol{f}\rangle \stackrel{\sim}{=} \lim_{\boldsymbol{\delta} \neq 0} \hat{\boldsymbol{g}}_{\boldsymbol{\delta}}^{-1/2} |N_{\boldsymbol{A}}, \boldsymbol{n}_{c}, \boldsymbol{f}\rangle.$$
(2.22)

The orthonormal vectors $|N_A, n_c, f\rangle^{\sim}$ are identified with physical states corresponding to $N(\alpha)$ composites in a single composite particle state corresponding to the state $|\alpha\rangle$ and $n(i), n(j), \ldots$ free or unbound elementary particles in states corresponding to the single elementary particle states $|i\rangle, |j\rangle, \ldots$ This definition appears reasonable, since the states in Eq. (2.22) are orthonormal and are as close as possible (in the mean square sense) to $|N_A, n_c, f\rangle$, which in turn were constructed to be physically close to what we mean by such composite particle states. Other definitions are possible but our definition has the virtues of simplicity and direct physical appeal.

The vectors $|N_A, n_c, f\rangle^{\sim}$ span the proper subspace P_c of \mathfrak{F} which can be made to approach \mathfrak{F} by allowing the cutoffs $\alpha_0, i_0, j_0, \ldots$ to become larger and larger. With the cutoffs sufficiently large we will take P_c to be the physical manybody space for all composite particle problems of interest. The vectors $|N_A, n_c, f\rangle^{\sim}$ then furnish us with a complete classification of many composite particle states within the frame work of nonrelativistic many-body theory. The cutoff represented by P_c is no real limitation of the theory. As was shown in SBG (appendix) a projector such as \hat{P}_c has the strong limit $1_{\mathfrak{F}}$ as the cutoff momenta are allowed to increase without limit.

III. COMPOSITE PARTICLE OCCUPATION NUMBER OPERATORS

Since the states $|N_A, n_c, f\rangle^{\sim} = |\{N(\alpha)\}, \{n(i)\}, \{n(j)\}, \dots, f\rangle^{\sim}$ given by Eq. (2.22) are orthonormal and by our definition have $N(\alpha)$ bound composites corresponding to the single composite particle state $|\alpha\rangle$, n(i) free elementary particles of type a corresponding to the single elementary particle state $|i\rangle, \dots$, we may use them to define a commuting set of composite number operators and free elementary particle operators. We define $\tilde{N}(\alpha)$, $\tilde{n}(i), \dots$, by means of

$$\tilde{N}(\alpha) | N_A, n_c, f \rangle^{\sim} \equiv N(\alpha) | N_A, n_c, f \rangle^{\sim}, \qquad (3.1)$$

$$\tilde{n}(i) |N_A, n_c, f\rangle^{\sim} \equiv n(i) |N_A, n_c, f\rangle^{\sim}, \qquad (3.2)$$

••• .

For completeness we may define $\tilde{N}(\alpha), \tilde{n}(i), \tilde{n}(j), \ldots$ to be zero on the orthogonal complement P_c^{\perp} of P_c in \mathfrak{F} , since we take P_c to be the Hilbert space of our many composite system. (We will modify this slightly in our treatment of statistical mechanics.)

If orthogonal projectors $\tilde{P}(N_A, n)$ are defined by

$$P(N_A, n) \equiv |N_A, n, f\rangle^{\sim \sim} \langle N_A, n, f|, \qquad (3.3)$$

then the operators $\tilde{N}(\alpha), \tilde{n}(i), \tilde{n}(j), \ldots$ may be written as

$$\tilde{N}(\alpha) = \sum_{N_A, n_c} N(\alpha) \tilde{P}(N_A, n) , \qquad (3.4)$$

$$\tilde{n}(i) = \sum_{N_A, n_c} n(i) \tilde{P}(N_A, n), \dots$$
(3.5)

The number operators $\tilde{N}(\alpha), \tilde{n}(i), \ldots$ are rather complicated objects, even though conceptually they are simply defined. We will show now that it is possible to express neatly the expression for $\tilde{N}(\alpha)$ by the introduction of creation and annihilation operators $\tilde{A}(\alpha)^*, \tilde{A}(\alpha)$, for which $\tilde{N}(\alpha)$ = $\tilde{A}(\alpha)^*\tilde{A}(\alpha)$. Further, on P_c these operators satisfy *elementary* Bose (Fermi) commutation (anticommutation) relations. The situation is much more complex for the operators $\tilde{n}(i)$, $\tilde{n}(j), \ldots$.

In the following, we make use of \hat{g}_{g} and will assume that in all expressions involving these operators the limit $\mathcal{E} \neq 0$ is taken. Then

$$\begin{split} |N_{A}, n_{c}, f\rangle^{\sim} &= \hat{g}_{\delta}^{-1/2} |N_{A}, N_{c}, f\rangle \\ &= g_{\delta}^{-1/2} \prod_{\alpha} \frac{[A(\alpha)^{*}]^{N(\alpha)}}{\sqrt{N(\alpha)!}} \hat{P}_{B}^{1} |n_{c}\rangle \\ &= \prod_{\alpha} \frac{[(\hat{g}_{\delta}^{-1/2} A(\alpha)^{*} \hat{g}_{\delta}^{1/2})]^{N(\alpha)}}{\sqrt{N(\alpha)!}} \hat{g}_{\delta}^{-1/2} \hat{P}_{B}^{1} |n_{c}\rangle \\ &\equiv \prod_{\alpha} \frac{[\tilde{A}(\alpha)^{*}]^{N(\alpha)}}{\sqrt{N(\alpha)!}} |0, n_{c}, f\rangle^{\sim}, \end{split}$$
(3.6)

where

$$[\bar{A}(\alpha)]^* \equiv \hat{g}_{\mathcal{S}}^{-1/2} A(\alpha)^* \hat{g}_{\mathcal{S}}^{1/2} . \qquad (3.6')$$

If
$$\tilde{A}(\alpha)^*$$
 is applied to $(N_A, n_c, f)^\sim$ we find that
 $\tilde{A}(\alpha_1)^* | N_A, n_c, f \rangle^\sim = \mathcal{E}(N_A) | \dots, N(\alpha_1) + 1, \dots, n_c, f \rangle^\sim$,
(3.7)

where $\mathcal{E}(N_A) = 1$ for boson composites and $\mathcal{E}(N_A) = (-1)^{\Sigma}$, $\sum \equiv \sum_{\alpha < \alpha_1} N(\alpha)$ for fermion composites. If $N(\alpha_1) = 1$ for fermion composites, of course $[\tilde{A}(\alpha_1)]^* | N_A, n, f \rangle^{\sim} = 0$. From Eq. (3.7) it is clear that the operators $\tilde{A}(\alpha)^*$ and $\tilde{A}(\alpha) \equiv [\tilde{A}(\alpha)^*]^*$ satisfy the following commutation or anticommutation relations:

$$\left[\tilde{A}(\alpha), \tilde{A}(\alpha')^*\right]_{\sharp} = \hat{P}_c \delta(\alpha, \alpha').$$
(3.8)

Furthermore, the composite particle number operators are expressed simply as

$$\tilde{N}(\alpha) = \tilde{A}(\alpha) * \tilde{A}(\alpha)$$
(3.9)

$$=\hat{g}_{\delta}^{-1/2}A(\alpha)*\hat{g}_{\delta}A(\alpha)\hat{g}_{\delta}^{-1/2}.$$
 (3.10)

It is noted that the maps

$$A(\alpha) - \tilde{A}(\alpha) = \hat{g}_{\delta}^{1/2} A(\alpha) \hat{g}_{\delta}^{-1/2}$$
, (3.11)

and

$$A(\alpha)^* - \tilde{A}(\alpha)^* = \hat{g}_{\delta}^{-1/2} A(\alpha)^* \hat{g}_{\delta}^{1/2}, \qquad (3.12)$$

are noncanonical: They transform the noncanonical

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operators $A(\alpha), A(\alpha)^*$ into canonical operators $\tilde{A}(\alpha), \tilde{A}(\alpha)^*$.

The presence of \hat{P}_{B}^{1} in the definition of $|N_{A}, n_{c}, f\rangle$ means that we cannot express $\tilde{n}(i), \ldots$ in such simple forms as $\tilde{N}(\alpha)$. That is, the $\tilde{n}(i), \tilde{n}(j), \ldots$ are more strongly many-body operators. The $\tilde{N}(\alpha)$ are also heavily dressed, but because of the structure of $|N_A, n_c, f\rangle^{\sim}$, they have a simpler construction. There has been some debate as to whether, for example, composite fermion or composite boson operators such as $\tilde{A}(\alpha), \tilde{A}(\alpha)^*$ could actually be constructed from elementary Bose and fermion operators. In Appendix B we present an explicit example where canonical ideal Bose composite operators are constructed from ideal Bose particle operators. The example there is very simple, but it illustrates the procedure. In order to construct composite fermions of course, elementary fermions are required.

IV. FOUNDATIONS OF STATISTICAL MECHANICS FOR COMPOSITE PARTICLES

Once occupation number operators for composite particles and free particles have been defined and constructed, the statistical mechanics of systems of such particles may be formulated directly. The state of such a many-body system is described in terms of the statistical operator $\hat{\rho}$, which satisfies the quantum Liouville equation

$$i\hbar\frac{d\hat{\rho}}{dt} = [\hat{H}, \hat{\rho}]. \tag{4.1}$$

In Eq. (4.1), \hat{H} is the full Hamiltonian operator for the many-body system and is expressed in terms of the elementary particle destruction and creation operators $a(i), a(i)^*, b(j), b(j)^*, \ldots$, corresponding to elementary particles of types a, b, \ldots . The expectation value $\langle O \rangle$ of any operator \hat{O} is given by the standard prescription

$$\langle \hat{O} \rangle = \operatorname{tr}(\hat{\rho}\hat{O}), \qquad (4.2)$$

where tr is the trace taken over a complete orthonormal set of states in F. The statistical operator is normalized to unity

 $\mathrm{tr}\,\hat{\rho}=1\,.\tag{4.3}$

The average number of composite particles in the state labeled by α is thus

$$\langle \tilde{N}(\alpha) \rangle = \operatorname{tr}[\hat{\rho}\tilde{N}(\alpha)],$$
(4.4)

where $\bar{N}(\alpha)$ is defined by Eq. (3.4) or (3.9). $\langle \tilde{N}(\alpha) \rangle$ changes with time according to

$$i\hbar \frac{d}{dt} \langle \tilde{N}(\alpha) \rangle = i\hbar \operatorname{tr} \left(\tilde{N}(\alpha) \frac{d\hat{\rho}}{dt} \right) = \operatorname{tr} \{ \tilde{N}(\alpha) [\hat{H}, \hat{\rho}] \},$$
(4.5)

etc.

In thermal equilibrium states the statistical operator is given by

$$\hat{\rho} = Z_G^{-1} \exp\left[-\beta(\hat{H} - \mu_a \tilde{N}_a - \mu_b \tilde{N}_b - \cdots)\right], \quad (4.6)$$

where $\beta = 1/kT$ and μ_a, μ_b, \ldots are chemical potentials for the elementary particles of types a, b, \ldots . Z_G is the grand partition function,

$$Z_{G} = \operatorname{tr} \exp[-\beta(\hat{H} - \mu_{a}\hat{N}_{a} - \mu_{b}\hat{N}_{b} - \cdots)]. \qquad (4.7)$$

The operators $\hat{N}_a, \hat{N}_b, \ldots$ are the total number operators for elementary particles of types a, b, \ldots ,

$$\hat{N}_{a} = \sum_{i} a(i) * a(i) ,$$
 (4.8)

$$\hat{N}_{b} = \sum_{j} b(j) * b(j), \dots$$
 (4.9)

The total number operator \tilde{N}_A for composite particles is defined by

$$\tilde{N}_{A} = \sum_{\alpha} \tilde{N}(\alpha) , \qquad (4.10)$$

where $\tilde{N}(\alpha)$ are given as before [Eq. (3.9)]. Rather than deal with *free* particle operators $\tilde{n}(i)$, etc., it is technically simpler to define the total number of free elementary particles through the operators $\tilde{N}_a^0, \tilde{N}_b^0, \ldots$, defined simply as follows: Let $l(a), l(b), \ldots$ be the number of elementary particles of type a, b, \ldots , which are present in the single composite particle state $|\alpha\rangle$; then

$$\hat{N}_a \equiv \tilde{N}_a^0 + l(a)\tilde{N}_A, \qquad (4.11)$$

$$\hat{N}_b \equiv \tilde{N}_b^0 + l(b)\tilde{N}_A, \qquad (4.12)$$

with $\hat{N}_a, \hat{N}_b, \ldots$ defined by Eqs. (4.8) and (4.9). Since \tilde{N}_A is constructed from products of elementary particle annihilation operators and the same number of elementary particle creation operators, \tilde{N}_A commutes with the commuting set $\{\hat{N}_a, \hat{N}_b, \ldots\}$ of operators. Therefore $\hat{N}_a, \hat{N}_b, \ldots, \tilde{N}_a^0, \tilde{N}_b^0, \ldots, \tilde{N}_A$ form a commuting set of number operators. However, \tilde{N}_A will, in general, not commute with the Hamiltonian, and therefore $\tilde{N}_a^0, \tilde{N}_b^0, \ldots$ also will not commute with the Hamiltonian. The definitions (4.11), (4.12),... may be employed in nonequilibrium situations. For the nonequilibrium case, since $\hat{N}_a, \hat{N}_b, \ldots$ commute with the Hamiltonian,

$$\frac{d}{dt}\langle \tilde{N}_{a}^{0}\rangle + l(a)\frac{d}{dt}\langle \tilde{N}_{A}\rangle = \frac{d}{dt}\langle \hat{N}_{a}\rangle = 0 , \qquad (4.13)$$

$$\frac{d}{dt}\langle \tilde{N}_b^0 \rangle + l(b)\frac{d}{dt}\langle \tilde{N}_A \rangle = \frac{d}{dt}\langle \hat{N}_b \rangle = 0, \dots, \qquad (4.14)$$

which relates the rates of increase of ionization of elementary particles to the rate of decrease of the number of bound composite particles.

In the equilibrium situation, the use of Eqs.

(4.11) and (4.12) in the grand partition function yields

$$Z_{G} = \operatorname{tr} \exp\left[-\beta(\hat{H} - \mu_{a}\tilde{N}_{a}^{0} - \mu_{b}\tilde{N}_{b}^{0} - \cdots - \mu_{a}\tilde{N}_{A})\right],$$
(4.15)

where

$$\mu_A \equiv l(a)\mu_a + l(b)\mu_b + \cdots, \qquad (4.16)$$

and the latter equation, Eq. (4.16), is just the thermodynamic relationship between the chemical potentials of the *free* elementary particles and *bound* composite particles. If we treat μ_A as an independent variable in Eq. (4.15), we may form the derivative $\partial Z_G / \partial \mu_A$, and obtain the result

$$\langle \bar{N}_{A} \rangle = kT \frac{\partial \ln Z_{G}}{\partial \mu_{A}}$$
(4.17)

for the equilibrium average number of composite particles, and where $kT = \beta^{-1}$ is the Boltzmann constant times the equilibrium Kelvin temperature T. It should be pointed out that \tilde{N}_a^0 defined above is not equal to $\sum_i \tilde{n}_a(i)$ in general. We feel that self-consistent definitions can be made, but we have not done so.

V. SEVERAL COMPOSITE TYPES

If the system is readily describable in terms of several bound composites (e.g., bound H, bound H₂), we must generalize the preceding procedures. Again let a, b, c, \ldots represent the types of elementary particles with $a(i), a(i)^*; b(j),$ $b(j)^*; \ldots$ their corresponding annihilation and creation operators. Let A, B, C, \ldots represent the types of bound composites with $A(\alpha), A(\alpha)^*; B(\beta), B(\beta)^*; \ldots$ their corresponding *single* composite annihilation and creation operators. Then single composite states in \mathfrak{F} are given by

$$|\alpha\rangle = A(\alpha)^* |0\rangle$$
, (5.1)

$$|\beta\rangle = B(\beta) * |0\rangle, \qquad (5.2)$$

where $\langle X | \alpha \rangle = \psi_{\alpha}(X), \langle Y | \beta \rangle = \psi_{\beta}(Y), \ldots$ are the (presumed known) wave functions for the single composites of types A, B, \ldots . As was emphasized in Sec. II, the choice of composites A, B, \ldots and single composite particle states $|\alpha\rangle, |\beta\rangle, |\gamma\rangle, \ldots$ depends upon conditions imposed upon the system as well as the processes to be described. These choices may be difficult but we assume that we have made these choices and know precisely the single composite particle states. The composite particle states must be independent, and it would not be acceptable to have, for example, any linear relation between the wave function $\psi_{\beta}(Y)$ and products $\psi_{\alpha}(X)\psi_{\alpha'}(X')$ of wave functions ψ_{α} .

We introduce vectors $|N, n_c, f\rangle$ analogous to the

vectors (N_A, n_c, f) defined in Eq. (2.20),

$$|N, n_{c}, f\rangle \equiv \prod_{\alpha, \beta, \dots} \frac{[A(\alpha)^{*}]^{N(\alpha)}}{\sqrt{N(\alpha)!}} \frac{[B(\beta)^{*}]^{N(\beta)}}{\sqrt{N(\beta)!}} \cdots \hat{P}_{B}^{1}|n_{c}\rangle,$$
(5.3)

the set $\{|n_c\rangle\}$ is a sub set of $\{|n\rangle\}$, the complete set of orthonormal vectors spanning F, chosen so as to make $\{|N, n_c, f\rangle\}$ linearly independent. The main point to be made here is that the vectors $|N, n_c, f\rangle$ must be linearly independent, which in turn depends upon suitable choices of $|\alpha\rangle$, $|\beta\rangle$, $|\gamma\rangle,\ldots$, and $\{|n_c\rangle\}$. The projector \hat{P}_B^1 is the projector onto the subspace orthogonal to all bound states. The construction of the vectors $|N, n_c, f\rangle$ cannot be a unique process. Physical considerations must be used in order to obtain the set appropriate to a given physical situation. That such a set $\{|N, n_c, f\rangle\}$ exists may be shown directly. For example, suppose boson composites of type Aare built up from two elementary particles and fermion composites of type B are built up from three elementary particles (for simplicity, all of the same type a). Let a^* stand for any elementary particle operator and consider the five- (elementary) particle subspace of F. Vectors of the form

(a) $A^*A^*a^*|0\rangle$

are linearly independent by the choice of the $|\alpha\rangle$. Vectors of the form

(b) $A^* \hat{P}^1_B a^* a^* a^* |0\rangle$

are linearly independent with vectors (a) and among themselves by choice of n_c . Vectors of the form

(c) $B^* \hat{P}_B^1 a^* a^* |0\rangle$

are linearly independent of vectors in (a) and (b) by choice of $B^*(\beta)$'s and among themselves by suitable choice of n_c . Vectors of the form

(d) $A^*B^*|0\rangle$

are linearly independent by choice of the A^* , B^* 's. Finally, vectors of the form $a^*a^*a^*a^*|0\rangle$ are complete in the five- (elementary) particle subspace, so we may choose a suitable set of vectors from these of type

(e) $\hat{P}_{B}^{1}a^{*}a^{*}a^{*}a^{*}a^{*}a^{*}|0\rangle$,

which are linearly independent among themselves and with vectors of types (a), (b), (c) and (d). [They are, of course, orthogonal to vectors of type (a), (b), (c), or (d).] We show in the Appendices how this may be done in a specific way. Thus we may take the vectors $|N, n_c, f\rangle$ to be linearly independent and total in \mathcal{F} .

Mathematically the problem appears to be

straightforward. We are given an overcomplete collection of vectors such as

$$\prod_{\alpha} A(\alpha)^* \prod_{\beta} B(\beta)^* \cdots \hat{P}_{\beta}^{\perp} \prod_{i} a(i)^* \prod_{j} b(j)^* \cdots |0\rangle$$
(5.4)

(no restrictions on i, j, \ldots) and we must select a complete linearly independent set which is then orthonormalized. One could carry out the selection one step at a time and use the Schmidt orthogonalization process. Mathematically one would arrive at a complete orthonormal collection of vectors. However, aside from the practical tedious details of actually carrying out the Schmidt process, the selection procedure is undemocratic, and gives greater weights to directions in F associated with earlier selections. Once the independent set has been selected on physical grounds, our procedure yields, using the des Cloizeaux orthogonalization method, an orthonormal set of states which closely resembles the physically selected vectors.

Once the vectors given by Eq. (5.3) have been determined, we may orthogonalize them. The resulting orthonormal set consists of the vectors

$$|N, n_c, f\rangle^{\sim} = \hat{g}_{\delta}^{-1/2} |N, n_c, f\rangle,$$
 (5.5)

where N stands for the set $\{N(\alpha), M(\beta), \dots\}$, $1 \le \alpha \le \alpha_0, \ 1 \le \beta \le \beta_0, \dots, \text{ and } n_c = \{n_a(i), n_b(j), \dots\}$, $i \le i \le i_0, \ 1 \le i \le i_0, \ 1 \le j \le j_0, \dots$, which are taken to represent states for which there are $N(\alpha)$ composites of type A in the single composite particle state $|\alpha\rangle, N(\beta)$ composites of type B in the single composite particle state $|\beta\rangle$, etc. The operator $\hat{g}_g = \mathbb{1}_g \hat{\mathcal{S}} + \hat{g}$ where

$$\hat{g} = \sum_{N,n_c} |N,n_c,f\rangle \langle N,n_c,f|.$$
(5.6)

Let l(A, a) be the number of elementary particles of type a in the single composite particle states of type A, l(A, b) the number of elementary particles of type b in the single composite particle states of type A, l(B, a) the number of elementary particles of type a in the single composite particle states of type B, etc. Then the number operators $\tilde{N}_a^0, \tilde{N}_b^0, \ldots$ for the total numbers of unbound (free) elementary particles are defined by

$$\sum_{i} a(i)^{*}a(i) = \hat{N}_{a} = \tilde{N}_{a}^{0} + l(A, a)\tilde{N}_{A} + l(B, a)\tilde{N}_{B} + \cdots,$$
(5.7)
$$\sum_{j} b(j)^{*}b(j) = \hat{N}_{b} = \tilde{N}_{b}^{0} + l(A, b)\tilde{N}_{A} + l(B, b)\tilde{N}_{B} + \cdots,$$
....

As in Sec. III, the operators \tilde{N}_A, \tilde{N}_B are given by

$$\tilde{N}_{A} = \sum_{\alpha} \tilde{N}(\alpha) ,$$

$$\tilde{N}_{B} = \sum_{\alpha} \tilde{N}(\beta) , \dots ,$$
(5.8)

where

. . . .

$$\tilde{N}(\alpha) |N, n_c, f\rangle^{\sim} \equiv N(\alpha) |N, n_c, f\rangle^{\sim},$$

$$\tilde{N}(\beta) |N, n_c, f\rangle^{\sim} \equiv N(\beta) |N, n_c, f\rangle^{\sim},$$
(5.9)

The grand partition function Z_G is now given by

$$Z_{G} = \operatorname{tr} \exp[-\beta(\hat{H} - \mu_{a}\hat{N}_{a} - \mu_{b}\hat{N}_{b} - \cdots)], \quad (5.10)$$

or, if we use Eqs. (5.7),

$$Z_G = \operatorname{tr} \exp\left[-\beta(\hat{H} - \mu_a \hat{N}_a^0 - \mu_b \hat{N}_b^0 - \cdots - \mu_A \tilde{N}_A - \mu_B \tilde{N}_B - \cdots)\right], \qquad (5.11)$$

where

$$\mu_{A} \equiv l(A, a)\mu_{a} + l(A, b)\mu_{b} + \cdots ,$$

$$\mu_{B} \equiv l(B, a)\mu_{a} + l(B, b)\mu_{b} + \cdots , \qquad (5.12)$$

As before, we may treat μ_A, μ_B, \ldots as independent variables in Eq. (5.11), so that

$$\beta \langle \vec{N}_A \rangle = \frac{\partial}{\partial \mu_A} \ln Z_G , \qquad (5.13)$$
$$\beta \langle \vec{N}_B \rangle = \frac{\partial}{\partial \mu_B} \ln Z_G , \dots .$$

The total numbers of unbound elementary particles then appear as

$$\beta \langle \tilde{N}_{a}^{0} \rangle = \frac{\partial}{\partial \mu_{a}} \ln Z_{G} , \qquad (5.14)$$
$$\beta \langle \tilde{N}_{b}^{0} \rangle = \frac{\partial}{\partial \mu_{b}} \ln Z_{G} , \dots .$$

Equations (5.13) and (5.14) can be regarded as fundamental equations which lead to generalized Saha-type equations.

The operators $\tilde{N}(\alpha), \tilde{M}(\beta), \tilde{n}(i), \tilde{n}(j), \ldots$ may be used in nonequilibrium situations where the state of the system is given by a time-dependent density operator $\hat{\rho}(t)$. Then the expectation values

$$\langle \tilde{N}(\alpha) \rangle_t = \operatorname{tr}[\hat{\rho}(t)\tilde{N}(\alpha)], \dots$$
 (5.15)

represent average number of composites in single composite particle states. This formalism thereby furnishes a basis for the statistical mechanics of interacting composite particles.

VI. CONCLUSION

A treatment of composite particles in nonrelativistic quantum many-body theory has been presented. The basic assumption made was that we have full knowledge of single composite particle states $|\alpha\rangle$, $|\beta\rangle$,.... For example, we may assume that wave functions $\psi_{\alpha}(X), \psi_{\beta}(Y), \psi_{\gamma}(Z), \ldots$ are given which correspond to single composite particles, and these may then provide the starting point of our treatment. Many-particle states are then introduced which correspond to arbitrary numbers $N(\alpha)$, $M(\beta)$, $O(\gamma)$,... of composite particles. These states reside in the elementary particle Fock space, so that exchange symmetry is always exact. Finally, creation and annihilation operators for composites are constructed as well as number operators for composites and free elementary particles. These number operators are then used to formulate the foundations of statistical mechanics for interacting composite particles.

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APPENDIX A: LINEAR INDEPENDENCE OF $|N,n_c|$

Let $a(i), a(i)^*, b(j), b(j)^*, \ldots$ be annihilation and creation operators for elementary particles of types a, b, \ldots corresponding to complete sets of orthonormal single particle states $|i\rangle, |j\rangle, \ldots$. Then as in Sec. II we may introduce a complete orthonormal set of vectors

$$|n\rangle = |n_a, n_b, \dots\rangle$$

=
$$\prod_{i, j, \dots, i} \frac{[a(i)^*]^{n(i)}}{[n(i)!]^{1/2}} \frac{[b(j)^*]^{n(j)}}{[n(j)!]^{1/2}} \dots |0\rangle.$$
(A1)

It is also convenient to work with vectors $|I\rangle$, where

$$|I\rangle = |i_1, \dots, j_1, \dots\rangle$$

= $\frac{1}{[N_a! N_b! \dots]^{1/2}} a(i_1) * a(i_2) * \dots |0\rangle$. (A2)

The index I includes N_a, N_b, \ldots , the numbers of the various elementary particles, as variables. The vectors $|I\rangle$ are complete in F,

$$\sum_{I} |I\rangle \langle I| = \mathbf{1}_{\mathfrak{F}}, \qquad (A3)$$

as are the vectors $|n\rangle$. The inner product $\langle I | I' \rangle$ is a Kronecker delta, symmetrized in the boson indices and antisymmetrized in the fermion indices. If $|A\rangle$ is any vector in \mathfrak{F} , we designate by $\Psi_A(I)$ the wave function corresponding to $|A\rangle$. If $|A\rangle$ has a definite number of elementary particles, $\Psi_A(I)$ will be zero for I not corresponding to the precisely prescribed number of variables in $|A\rangle$. If $\langle A | A \rangle = 1$, then

$$\sum_{I} \overline{\Psi}_{A}(I) \Psi_{A}(I) = 1 , \qquad (A4)$$

or if we use continuous I variables,

$$\int dI \,\overline{\Psi}_{A}(I) \Psi_{A}(I) = 1 \,. \tag{A5}$$

Since the vectors $|I\rangle$ span the entire Fock space \mathfrak{F} , the vectors $A(\alpha)^*|I\rangle$ and $|I\rangle$ cannot be linearly independent. The set $\{|I\rangle\}$ of vectors $|I\rangle$ may be considered linearly independent in the sense that if $\sum C_I |I\rangle = 0$, and if the coefficients C_I are antisymmetric in fermion indices and symmetric in boson indices, then $C_I \equiv 0$. In the following discussion of linear independence, all coefficients C_I are assumed to possess this symmetry.

We introduce cutoffs $\alpha_0, \beta_0, \ldots$ in the composite particle states and i_0, j_0, \ldots in the elementary particle states. The labels α , etc., are ordered, $1 \le \alpha \le \alpha_0, \ \alpha = 1, 2, 3, \ldots; \ i = 1, 2, 3, \ldots, i_0; \ j$ $= 1, 2, 3, \ldots, j_0; \ldots$ The collection of such elementary particle labels is called $\{J\} \subset \{I\}$, so that $J \in \{J\}$ means $J = (i_1, \ldots, i_r; j_1, \ldots, j_r; \ldots), \ i_k \le i_0, \ j_1 \le j_0$, etc.

The basic technical assumption concerning $|\alpha\rangle$, $|\beta\rangle$,... is that $\Psi_{\alpha}(I) = \langle I | \alpha \rangle$ have no cutoff in i_1, \ldots, j_1, \ldots . It then follows from a mild assumption that $|J\rangle$ and $A(\alpha)^* | J \rangle$ are linearly independent. Let, for fixed α ,

$$\sum_{J} C_{J} |J\rangle + \sum_{J} C_{\alpha J} A(\alpha) * |J\rangle = 0 , \qquad (A6)$$

then

$$A(\alpha) * \sum_{J} C_{\alpha J} |J\rangle = -\sum_{J} C_{J} |J\rangle$$

so $A(\alpha)^* \sum_J C_{\alpha J} |J\rangle$ lies entirely in the subspace P_c spanned by $\{|J\rangle\}$. Hence by our requirement that $A(\alpha)^*$ have no cutoff in *I*, the only vector $|\psi\rangle$ for which $A(\alpha)^* |\psi\rangle$ is in P_c is $|\psi\rangle = 0$, so that

$$\sum_{J} C_{\sigma J} \left| J \right\rangle = 0 , \qquad (A7)$$

and by the linear independence of $\{|J\rangle\}$,

$$C_{\alpha I} = 0. \tag{A8}$$

Therefore

$$\sum_{J} C_{J} |J\rangle = 0$$

and

$$C_J = 0$$

so the vectors $|J\rangle$, $A(\alpha)^*|J\rangle$, $J \in \{J\}$ are linearly independent for a given α . Next we show that $|J\rangle$, $A(\alpha)^*|J\rangle$ are linearly independent for $1 \le \alpha \le \alpha_0$. Let

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(A9)

$$\sum_{J} C_{J} |J\rangle + \sum_{\alpha, J} C_{\alpha J} A(\alpha) * |J\rangle = 0 , \qquad (A10)$$

and write $|K\rangle \equiv \mathfrak{A}_{K}^{*}|0\rangle$, where K has none of its indices equal to any of those of any J. Then if we multiply Eq. (A10) by \mathfrak{A}_{K} , where K has the same number of indices of each type as J, we have

$$\sum_{\alpha J} C_{\alpha J} \mathfrak{A}_{K} A(\alpha)^{*} | J \rangle = 0 , \qquad (A11)$$

since $\alpha_{\kappa} |J\rangle = 0$. By Wick's theorem

$$\mathfrak{A}_{\kappa}A(\boldsymbol{\alpha})^{*}|J\rangle = \psi_{\boldsymbol{\alpha}}(K)|J\rangle,$$

since only the complete contractions of \mathcal{C}_K with $A(\alpha)^*$ survive. Therefore from Eq. (A11) we have

$$\sum_{J} \sum_{\alpha} C_{\alpha J} \psi_{\alpha}(K) | J \rangle = 0 .$$
 (A12)

The $|\mathcal{J}\rangle$ are linearly independent, so the coefficient of $|\mathcal{J}\rangle$ is zero:

$$\sum_{\alpha=1}^{\alpha_0} C_{\alpha J} \psi_{\alpha}(K) = 0 , \qquad (A13)$$

 $\{K\} \cap \{J\} = \phi$. The wave functions $\psi_{\alpha}(I)$ are linearly independent and since there are an infinite number of equations [Eq. (A13)] and only a finite number of α 's, we make the reasonable technical assumption that $\psi_{\alpha}(K)$ are also linearly independent. Hence

$$C_{\alpha I} = 0. \tag{A8}$$

Therefore Eq. (A10) yields

 $\sum_{J} C_{J} \left| J \right\rangle = 0 ,$

and $C_J = 0$. Therefore $|J\rangle$ and $A(\alpha)^*|J\rangle$ are linearly independent.

We now proceed by induction to prove that $A(\alpha_1)^*A(\alpha_2)^*\cdots A(\alpha_r)^*|J\rangle$, $0 \le r \le M$ are linearly independent in the sense that

$$0 = \sum_{r,\alpha_1,\ldots,\alpha_r \ J} C_{\alpha_1} \cdots_{\alpha_r \ J} A(\alpha_1)^* \cdots A(\alpha_1)^* |J\rangle,$$
(A14)

where $C_{\alpha_1} \cdots \alpha_r J$ has composite boson or fermion symmetry with respect to the indices α , implies C=0. Multiply Eq. (A14) by α_{KM} , where *M* indicates that α_{KM} has precisely the same number of elementary particle destruction operators as $A(\alpha_1)^* \cdots A(\alpha_M)^*$ has creation operators. Then

$$0 = \sum_{\alpha_1 \cdots \alpha_M J} C_{\alpha_1 \cdots \alpha_M J} \mathcal{Q}_{KM} A(\alpha_1)^* \cdots A(\alpha_M)^* | J \rangle,$$
(A15)

and by the same argument as before only the completely contracted terms of \mathcal{C}_{KW} with $A(\alpha_1)^*, \ldots$, $A(\alpha_M)^*$ survive. Hence the linear independence of the $|J\rangle$'s yields

$$0 = \sum_{\alpha_1 \cdots \alpha_M J} \left[S(\psi_{\alpha_1}(K_1) \cdots \psi_{\alpha_M}(K_M)) \right] C_{\alpha_1 \cdots \alpha_M J},$$
(A16)

where $K = (K_1, K_2, \ldots, K_M)$, and S antisymmetrizes fermion indices in the K and symmetrizes the boson indices in the K. Even though the $\psi_{\alpha}(K)$ are orthonormal, the $S(\psi_{\alpha_1} \cdots \psi_{\alpha_M})$ in general are not. Again the sum over α 's is finite and Eq. (A16) holds for an infinite number of K's, and we assume that $(S\psi_{\alpha_1} \cdots \psi_{\alpha_M})(K)$ are linearly independent. Hence

$$C_{\alpha_1\cdots\alpha_M J} = 0. \tag{A17}$$

We have therefore shown that

$$0 = \sum_{r=i}^{m-1} \sum_{\alpha_1,\ldots,\alpha_r} \sum C_{\alpha_1}\cdots_{\alpha_r} A(\alpha_1)^*\cdots A(\alpha_r)^* |J\rangle,$$
(A18)

and by our inductive assumption, $C_{\alpha_1 \cdots \alpha_r} = 0$. Therefore the vectors

 $A(\alpha_1)^* \cdots A(\alpha_N)^* |J\rangle$

.

are linearly independent, $M = 0, 1, 2, \ldots$.

The case for several composites is treated quite similarly. Several additional requirements are necessary. For example, we cannot allow a composite $|B\rangle = B(\beta) * |0\rangle$ to be expressible as

$$B(\beta)^* = \sum_{\alpha_1 \alpha_2 = 0}^{\alpha_0} C_{\beta \alpha_1 \alpha_2} A(\alpha_1)^* A(\alpha_2)^*.$$
 (A19)

Consider two distinct types of composites A, Bwith single composite states $|\alpha\rangle = A(\alpha)^* |0\rangle$ and $|\beta\rangle = B(\beta)^* |0\rangle$. We will show, under certain mild conditions, that the vectors

$$|r, s, J\rangle \equiv A(\alpha_1)^* \cdots A(\alpha_r)^* B(\beta_1)^* \cdots B(\beta_s)^* |J\rangle$$
(A20)

are linearly independent. By the previous argument $|r, 0, J\rangle$ are linearly independent and $|0, s, J\rangle$ are linearly independent. We make the technical assumption that the combined set consisting of both types $|r, 0, J\rangle$ and $|0, s, J\rangle$ are also linearly independent. This only means that the states $|\alpha\rangle$ and $|\beta\rangle$ have been chosen so that there is no linear relation between $A(\alpha_1)^* \cdots A(\alpha_r)^* |J\rangle$ and $B(\beta_1)^* \cdots B(\beta_s)^* |J\rangle$, even when it turns out that these two sets of vectors have the same numbers of elementary particles. We partially order the given vectors by a number N, which orders the number of elementary particles, and proceed by induction. Any zero linear relation among vectors having N or less elementary particles yields upon operating on that linear relation by $\mathbf{a}_{N}(K)$ the following:

$$\sum_{r,s} \sum_{(\alpha)(\beta)} C_{r,s}^{(N)}(\alpha_1,\ldots,\alpha_r;\beta_1,\ldots,\beta_s;J) \mathfrak{a}_N(K) A(\alpha_1)^* \cdots A(\alpha_r)^* B(\beta_1)^* \cdots B(\beta_s)^* |J\rangle = 0, \qquad (A21)$$

where the sum on r, s is such that all vectors corresponding to N elementary particles are included. Wick's theorem then yields, since the $|J\rangle$ are linearly independent,

$$0 = \sum_{r,s} \sum_{(\alpha)(\beta)} C_{rs}^{(N)}(\alpha_1, \dots, \alpha_r; \beta_1, \dots, \beta_s; J) S(\psi_{\alpha_1}(K_1), \dots, \psi_{\alpha_r}(K_r); \psi_{\beta_1}(K_1'), \dots, \psi_{\beta_s}(K_s')).$$
(A22)

Again (A22) represents an infinite number of relations (all K corresponding to N elementary particles), and we assume the finite set of wave functions $\psi_{\alpha}, \psi_{\beta}$ to be such that these $(S\psi)(K)$ are linearly independent. Therefore all $C_{rs}^{(N)}(\alpha_1, \ldots, \alpha_r; \beta_1, \ldots, \beta_s; J) = 0$, N fixed.

Our inductive assumption then implies $C_{rs}^{(R)}(\alpha_1, \ldots, \alpha_r; \beta_1, \ldots, \beta_s; J) = 0$ for R < N, and thus the vectors given by Eq. (A20) are linearly independent. The argument for more composite types is similar.

APPENDIX B: A SIMPLE EXAMPLE

Since the procedures outlined in Sec. II are somewhat abstract, we show by means of a very simple example how the method works. Let a, bbe two Bose destruction operators corresponding to two bosons, each of which has only one single particle state. The normalized vector

$$|n_1, n_2\rangle = \frac{1}{(n_1! \, n_2! \,)^{1/2}} \, (a^*)^{n_1} (b^*)^{n_2} \, |0\rangle \tag{B1}$$

represents a state which has n_1 bosons of type a and n_2 bosons of type b.

We introduce the *composite* boson operators A = ab, $A^* = a^*b^*$, so that

$$[A, A^*] = 1 + a^*a + b^*b , \qquad (B2)$$

$$[a, A^*] = b , \tag{B3}$$

etc.

Introduce next the vectors

$$|N,n_c\rangle \equiv \frac{(A^*)^N}{(N!)^{1/2}} \, \frac{(a^*)^n}{(n!)^{1/2}} \, |0\rangle \,, \tag{B4}$$

or

$$|N, n_c\rangle = \left(\frac{(n+N)!}{n!}\right)^{1/2} |N+n,N\rangle.$$
 (B5)

The self-adjoint operator \hat{g} is then

$$\hat{g} = \sum_{n,N} \frac{(n+N)!}{n!} \hat{P}(N+n,N), \qquad (B6)$$

where $\hat{P}(N, n, N)$ is the projector on the one-dimensional subspace spanned by $|N+n,N\rangle$. If \hat{g} is restricted to the subspace P_c spanned by the vectors given by Eq. (B4),

$$\hat{g}^{-1/2} = \sum_{N,n} \left(\frac{n!}{(N+n)!} \right)^{1/2} \hat{P}(N+n,N)$$

and the vectors $|N,n\rangle^{\sim} = \hat{g}^{-1/2} \langle N,n_c \rangle$ are just

$$|N,n\rangle^{\sim} = |N+n,N\rangle \tag{B7}$$

and

and

$$\hat{P}_{c} = \sum_{N,n} |N,n\rangle^{\sim} \langle N,n|^{\sim} = \sum_{N,n} \hat{P}(N+n,N).$$
(B8)

The destruction operator for the *free* boson \tilde{a} is given by

$$\tilde{a} = \hat{g}^{1/2} a \hat{g}^{-1/2}$$
$$= \sum_{N,n} \sqrt{n+1} |N+n, N\rangle \langle N+n, N|.$$
(B9)

Similarly the destruction operator for the *bound* boson \bar{A} is given by

$$\tilde{A} = \sum_{N,n} \sqrt{N+1} |N+n, N\rangle \langle N+n+1, N+1|.$$
(B10)

It is a simple computation to show that

$$\begin{bmatrix} \tilde{a}, \tilde{a}^* \end{bmatrix} = \sum_{N,n} \hat{P}(N+n, N) = \hat{P}_c,$$

$$\begin{bmatrix} \tilde{A}, \tilde{A}^* \end{bmatrix} = \hat{P}_c,$$

$$\begin{bmatrix} \tilde{a}, \tilde{A} \end{bmatrix} = \begin{bmatrix} \tilde{a}, \tilde{A}^* \end{bmatrix} = \begin{bmatrix} \tilde{a}^*, \tilde{A} \end{bmatrix} = 0,$$
(B11)

so that \tilde{a}, \tilde{A} are simple Bose destruction operators on P_c . The commuting number operators for \tilde{a}, \tilde{A} are

$$\tilde{n} = \tilde{\alpha}^* \tilde{\alpha} = \sum_{N,n} n \hat{P}(N+n,N)$$

$$\tilde{N} = \tilde{A}^* \tilde{A} = \sum_{N,n} N \hat{P}(N+n,N) .$$
(B12)

Even though this is a very simple example compared to any realistic many-body problem, it shows that the bare operators a, A = ab, must be *heavily dressed* to produce \tilde{a}, \tilde{A} , which satisfy *strict* elementary Bose commutation relations on P_a . We note that, for example,

$$\tilde{A} = \sum_{N,n} \sqrt{N+1} \frac{1}{[(N+n)!N!]^{1/2}} (a^*)^{N+n} (b^*)^N \hat{P}_0$$
$$\times (b)^{N+1} (a)^{N+n+1} \frac{1}{[(N+1)!(N+n+1)!]^{1/2}} , \quad (B13)$$

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where $\hat{P}_0 = |0,0\rangle\langle 0,0|$. In order to express \tilde{A} solely in terms of a, b, a^*, b^* , we must so express \hat{P}_0 :

$$\hat{P}_0 = :e^{-(a^*a + b^*b)}:$$
 (B14)

$$\equiv \sum_{n_1 n_2} (-1)^{n_1 + n_2} \frac{1}{n_1! n_2!} (a^*)^{n_1} (b^*)^{n_2} (b)^{n_2} (a)^{n_1}, \quad (B15)$$

so \tilde{A} is a fairly complicated operator in terms of a, a^*, b, b^* . We observe that the number operators \tilde{n} and \tilde{N} , besides commuting with each other, commute with the bare Bose number operators a^*a and b^*b .

APPENDIX C: LINEAR INDEPENDENCE OF $|N,n_c, f\rangle$

For convenience, we restrict our considerations to composites (atoms) made up from a single species of elementary fermions and each atom consists of only two elementary particles. Let

$$\hat{g}(N) = \sum_{\substack{\mathbf{r}, \mathbf{s} \geq 0\\ 2\mathbf{r} + \mathbf{s} = \mathbf{N}}} |\alpha_1 \cdots \alpha_{\mathbf{r}} i_1 \cdots i_s f\rangle \langle \alpha_1 \cdots \alpha_{\mathbf{r}} i_1 \cdots i_s f|$$
$$\equiv |i_1 \cdots i_N f\rangle \langle i_1 \cdots i_N f| + \hat{g}_B(N) , \qquad (C1)$$

where

$$\begin{aligned} |\alpha_{1}\cdots\alpha_{r} i_{1}\cdots i_{s} f\rangle \\ &= \frac{1}{(r! s!)^{1/2}} A(\alpha_{1})^{*} A(\alpha_{2})^{*}\cdots A(\alpha_{r})^{*} \\ &\times \hat{P}_{B}^{1}(s) a(i_{1})^{*}\cdots a(i_{s})^{*} |0\rangle \\ &= \frac{1}{(r!)^{1/2}} A(\alpha_{1})^{*}\cdots A(\alpha_{r})^{*} \hat{P}_{B}^{1}(s) |i_{1}\cdots i_{s}\rangle. \end{aligned}$$
(C2)

where

$$|\widetilde{\alpha}_j| \leq k_c, \quad j=1,\ldots,r$$

 $|\widetilde{\mathbf{i}}_j| \leq k_c, \quad j=1,\ldots,s$

and

$$\hat{P}_{B}^{1}(s)|\psi\rangle = |\psi\rangle$$
 if and only if $\hat{g}_{B}(s)|\psi\rangle = 0$. (C3)

We will show that the states, $|\alpha_1 \cdots \alpha_r i_1 \cdots i_s f\rangle$, are linearly independent, outside of the trivial permutational linear dependence, i.e., that

$$\sum_{2r+s=N} \sum_{\substack{\alpha_1\cdots\alpha_r\\i_1\cdots i_s}} |\alpha_1\cdots\alpha_r, i_1\cdots i_s\rangle \times C(\alpha_1,\ldots,\alpha_r; i_1,\ldots,i_s) = 0, \quad (C4)$$

implies $C(\alpha_1, \ldots, \alpha_r; i_1, \ldots, i_s) = 0$, where the C's are symmetric in the α 's and antisymmetric in the *i*'s.

The proof depends upon the skew-symmetric products of the bound state wave functions being linearly independent. This in turn depends upon the mild technical assumption that the interatom exchange operators cannot be expressed solely in terms of the bound state wave functions, which are not complete. For example, for four particles,

$$\sum_{P} \varphi_{\alpha_{1}}(i_{P_{1}}, i_{P_{2}})\varphi_{\alpha_{2}}(i_{P_{3}}, i_{P_{4}})\delta_{P} = (2!)^{2} [\varphi_{\alpha_{1}}(i_{1}, i_{2})\varphi_{\alpha_{2}}(i_{3}, i_{4}) + \varphi_{\alpha_{1}}(i_{1}, i_{4})\varphi_{\alpha_{2}}(i_{2}, i_{3}) + \varphi_{\alpha_{1}}(i_{1}, i_{3})\varphi_{\alpha_{2}}(i_{2}, i_{4}) + (\alpha_{1} \leftrightarrow \alpha_{2})] \neq \sum_{\alpha, \alpha'} \varphi_{\alpha}(i_{1}, i_{2})\varphi_{\alpha'}(i_{3}, i_{4})C(\alpha, \alpha').$$
(C5)

As a consequence, then, there is no way to satisfy

$$\sum_{\alpha_1,\alpha_2} \sum_{P} \delta_P \varphi_{\alpha_1}(i_{P_1}, i_{P_2}) \varphi_{\alpha_2}(i_{P_3}, i_{P_4}) C(\alpha_1, \alpha_2) = 0.$$
(C6)

For all values of i_1, i_2 ; $|\vec{1}| > k_c$, except $C(\alpha_1, \alpha_2) = 0$ [of course, $C(\alpha_1, \alpha_2) = C(\alpha_2, \alpha_1)$]. The last term in (C5) cannot be restricted to the bound states alone, but must include four scattering states. For general, r, then we assume

$$\sum_{P} \delta_{P} \varphi_{\alpha_{1}}(i_{P_{1}}, i_{P_{2}}) \varphi_{\alpha_{2}}(i_{P_{3}}, i_{P_{4}}) \cdots \varphi_{\alpha_{r}}(i_{P(2r-1)}, i_{P(2r)}) \neq \sum_{\alpha_{1}' \cdots \alpha_{r}'} A(\alpha_{1}' \cdots \alpha_{r}') \varphi_{\alpha_{1}'}(i_{1}, i_{2}) \varphi_{\alpha_{2}'}(i_{3}, i_{4}) \cdots \varphi_{\alpha_{r}'}(i_{2r-1}, i_{2r}),$$
(C7)

where the sum is restricted to bound states only.

To proceed with the proof we can realize (C4) as

$$\sum_{2r+s=N} \sum_{(\alpha)(i)} |\alpha_1 \cdots \alpha_r i_1 \cdots i_s f\rangle C(\alpha_1, \dots, \alpha_r; i_1, \dots, i_s) = \sum_{2r+s=N} \sum_{(\alpha)(i)} |\alpha_1 \cdots \alpha_r i_1 \cdots i_s\rangle \overline{C}(\alpha_1, \dots, \alpha_r; i_1, \dots, i_s), \quad (C8)$$

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where

$$|\alpha_1 \cdots \alpha_r \ i_1 \cdots i_s\rangle = (1/\sqrt{r!})A(\alpha_1)^*A(\alpha_2)^* \cdots A(\alpha_r)^* |i_1 \cdots i_s\rangle, \quad |\vec{\alpha}_j| \le k_c, \quad |\vec{1}_j| \le k_c$$
(C9)

which differs from (C2) by the absence of P_B^{\perp} .

We shall first show the \overline{C} 's are zero. Assume N even and take the inner product of (C7) with $|i_1 \cdots i_N\rangle$ where all $|\vec{i}_K| > k_c$. Then

$$\sum_{(\alpha)} \frac{1}{[N!(\frac{1}{2}N)!]^{1/2}} \sum_{P} \delta_{P} \varphi_{\alpha_{1}}(i_{P_{1}}, i_{P_{2}}) \cdots \varphi_{\alpha_{N/2}}(i_{P(N-1)}, i_{P_{N}}) \overline{C}(\alpha_{1}, \dots, \alpha_{N/2}) = 0.$$
(C10)

By the linear independence of the skew-symmetric states and the symmetry of the \overline{C} 's, $\overline{C}(\alpha_1, \ldots \alpha_{N/2}) = 0$. The remainder follows by induction. Assume $\overline{C} = 0$ for $r > r_0$. Take the inner product of (C7) with $|i_1 \cdots i_N\rangle$ where $|\overline{i}_k| > k_c$, $k = 1, \ldots, 2r_0$, and $|\overline{i}_k| \le k_c$, $k = 2r_0 + 1, \ldots, N$. One then obtains

$$\sum_{\substack{r \leq r_0 \\ 2r+s = N}} \sum_{(\alpha)(i)} \sum_{P} \delta_{P} \frac{1}{(r!s!N!)^{1/2}} \varphi_{\alpha_{1}}(i_{P_{1}}, i_{P_{2}}) \cdots \varphi_{\alpha_{r}}(i_{P_{2r-1}}, i_{P_{2r}}) C(\alpha_{1}, \dots, \alpha_{r}; i_{P_{2r+1}}, \dots, i_{P_{N}})$$

$$= \sum_{(\alpha)} \sum_{P} \delta_{P} \frac{(N-2r_{0})!}{[r_{0}!(N-2r_{0})!]^{1/2}} \varphi_{\alpha_{1}}(i_{P_{1}}, i_{P_{2}}) \cdots \varphi_{\alpha_{r_{0}}}(i_{P_{2r_{0}-1}}, i_{P_{2r_{0}}}) \overline{C}(\alpha_{1}, \dots, \alpha_{r_{0}}; i_{2r_{0}+1}, \dots, i_{N}) = 0. \quad (C11)$$

Again by linear independence, and the symmetry properties of \overline{C} , $\overline{C}(\alpha_1, \ldots, \alpha_{r_0}; i_1, \ldots, i_{N-2r_0}) = 0$, and hence all \overline{C} 's are zero. The case N = odd is proven similarly, except that the states, $|i_1 \cdots i_N\rangle$, have odd numbers of *i*'s with $|\overline{i}|$ in each step of the proof.

We now return to the problem of proving (C8) by explicitly relating the \overline{C} 's to the C's and showing that all $\overline{C} = 0$ implies all C = 0. We observe

$$\hat{P}_{B}(s)^{\perp} |i_{1}\cdots i_{s}\rangle = |i_{1}\cdots i_{s}\rangle - \hat{g}_{B}(s)[\mathcal{E}\mathbf{1} + \hat{g}_{B}(s)]^{-1} |i_{1}\cdots i_{s}\rangle$$

$$= |i_{1}\cdots i_{s}\rangle - \sum_{\substack{\overline{\tau}>0\\2\overline{\tau}+\overline{s}=s}} \sum_{(\overline{\alpha})(\overline{\iota})} \frac{1}{\sqrt{\overline{\tau}!}} A(\overline{\alpha}_{1})^{*}\cdots A(\overline{\alpha}_{\overline{s}})^{*} \hat{P}_{B}^{\perp}(\overline{s}) |\overline{i}_{1}\cdots \overline{i}_{\overline{s}}\rangle$$

$$\times \langle \overline{i}_{1}\cdots \overline{i}_{\overline{s}} | (\hat{g}_{B}(s) + \mathcal{E})^{-1} | i_{1}\cdots i_{s}\rangle.$$
(C12)

One can similarly expand $\hat{P}_{B}^{1}(\overline{s})|(\overline{i})\rangle$ in terms of $\hat{P}_{B}^{1}(\underline{s})i_{1}\cdots i_{s}\rangle$, etc., so that we eventually obtain

$$\hat{P}_{B}^{\perp}(s)|i_{1}\cdots i_{s}\rangle = |i_{1}\cdots i_{s}\rangle - \sum_{2\overline{\tau}+\overline{s}=N} \sum_{(\overline{\alpha})(\overline{i})} |\overline{\alpha}_{1}\cdots\overline{\alpha}_{\overline{\tau}},\overline{i}_{1}\cdots\overline{i}_{\overline{s}}\rangle D_{s}(\overline{\alpha}_{1},\ldots,\overline{\alpha}_{\overline{\tau}};\overline{i}_{1},\ldots,\overline{i}_{\overline{s}}|i_{1},\ldots,i_{s}), \quad (C13)$$

where D_s 's are coefficients symmetric in the α 's and antisymmetric in $\overline{i_1}, \ldots, \overline{i_s}$ and i_1, \ldots, i_s . Specifically,

$$\hat{P}_{B}^{1}(0)\left|0\right\rangle = \left|0\right\rangle,\tag{C14}$$

$$\hat{P}_{B}^{1}(1)|i\rangle = |i\rangle, \qquad (C15)$$

$$\hat{P}_{B}^{1}(2)|i_{1}i_{2}\rangle = |i_{1}i_{2}\rangle - \sum_{\alpha} |\alpha\rangle\langle\alpha|i_{1}i_{2}\rangle, \qquad (C16)$$

$$\hat{P}_{B}^{1}(3)|i_{1}i_{2}i_{3}\rangle = |i_{1}i_{2}i_{3}\rangle - \sum_{\alpha,i} |\alpha,i\rangle\langle\alpha,i|\frac{1}{\hat{g}_{B}(3) + \mathcal{E}1}|i_{1}i_{2}i_{3}\rangle , \qquad (C17)$$

$$\hat{P}_{B}^{1}(4) |i_{1}i_{2}i_{3}i_{4}\rangle = |i_{1}i_{2}i_{3}i_{4}\rangle - \sum_{\alpha i_{1}i_{2}} |\alpha i_{1}i_{2}\rangle \langle \alpha i_{1}i_{2} | \hat{g}_{B}^{-1}(3) | i_{1}i_{2}i_{3}\rangle \\ - \sum_{\alpha_{1}\alpha_{2}} |\alpha_{1}\alpha_{2}\rangle [\langle \alpha_{1}\alpha_{2} | \hat{g}_{B}^{-1}(3) | i_{1}i_{2}i_{3}i_{4}\rangle - \langle \alpha_{2}i_{1}i_{2}\rangle \langle \alpha_{1}i_{1}i_{2}f | \hat{g}_{B}^{-1}(4) | i_{1}\cdots i_{4}\rangle].$$
(C18)

As a consequence of (C12),

$$\alpha_{1}\cdots\alpha_{r}\ i_{1}\cdots i_{s}\ f\rangle \equiv (1/\sqrt{r!}\)A(\alpha_{1})^{*}\cdots A(\alpha_{r})^{*}\ |i_{1}\cdots i_{s}\ f\rangle$$
$$= |\alpha_{1}\cdots\alpha_{r}\ i_{1}\cdots i_{s}\rangle - \sum_{\substack{2\overline{r}+\overline{s}=s\\\overline{r}>0,\overline{s}>0}}\sum_{(\overline{\alpha})(\overline{i})} \left(\frac{(r+\overline{r})!}{r!\overline{r}!}\right)^{1/2} |\alpha_{1}\cdots\alpha_{r}\ \overline{\alpha}_{1}\cdots\overline{\alpha}_{\overline{r}}\ \overline{i_{1}}\cdots\overline{i_{s}}\rangle D_{s}((\overline{\alpha})(\overline{i})(i)).$$
(C19)

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Thus,

$$\sum_{\substack{\alpha_{1}\cdots\alpha_{r}\\i_{1}\cdots i_{s}}} |\alpha_{1}\cdots\alpha_{r}i_{1}\cdots i_{s}f\rangle C(\alpha_{1},\ldots,\alpha_{r};i_{1},\ldots,i_{s})$$

$$= \sum_{\substack{(\alpha)(i)}} |\alpha_{1}\cdots\alpha_{r}i_{1}\cdots i_{s}\rangle C(\alpha_{1},\ldots,\alpha_{r};i_{1},\ldots,i_{s})$$

$$- \sum_{\underline{2r}+\overline{s}=s} \left(\frac{(r+\overline{r})!}{r!\,\overline{r}!}\right)^{\frac{1}{2}} \sum_{(\alpha)(\overline{\alpha})(i)(\overline{i})} D_{S}(\overline{\alpha}_{1},\ldots,\overline{\alpha}_{\overline{r}};\overline{i}_{1},\ldots,\overline{i}_{\overline{s}};i_{1},\ldots,i_{s}) C(\alpha_{1},\ldots,\alpha_{r};i_{1},\ldots,i_{s})$$

$$\equiv \sum_{\substack{R \ge r\\2R+\overline{s}=N}} \sum_{(\overline{\alpha})(\overline{i})} |\overline{\alpha}_{1}\cdots\overline{\alpha}_{R}\,\overline{i}_{1}\cdots\overline{i}_{\overline{s}}\rangle \tilde{C}_{r}(\overline{\alpha}_{1},\ldots,\overline{\alpha}_{R};\overline{i}_{1},\ldots,\overline{i}_{\overline{s}}), \qquad (C20)$$

where

$$\tilde{C}_{r}(\overline{\alpha}_{1},\ldots,\overline{\alpha}_{R};\overline{i}_{1},\ldots,\overline{i}_{s}) = \begin{cases} C(\overline{\alpha}_{1},\ldots,\overline{\alpha}_{r};\overline{i}_{1},\ldots,\overline{i}_{N-2r}), & R=r \\ \frac{-1}{[R|r!(R-r)!]^{1/2}} \sum_{P} \sum_{i_{1}\cdots i_{s}} C(\overline{\alpha}_{P_{1}},\ldots,\overline{\alpha}_{P_{R}};i_{1},\ldots,i_{s}) \\ \times D_{s}(\overline{\alpha}_{P_{r+1}},\ldots,\overline{\alpha}_{P_{R}};\overline{i}_{1},\ldots,\overline{i}_{s}|i_{1},\ldots,i_{s}), & R>r \end{cases}$$
(C21)

where P is the permutation of R atoms. Thus

$$\sum_{(\alpha)(i)} \sum_{2r+s=N} |\alpha_1 \cdots \alpha i_1 \cdots i_s f\rangle C(\alpha_1, \dots, \alpha; i_1, \dots, i_s)$$

$$= \sum_{r \ge 0, R \ge r, 2R+\overline{s}=N} \sum_{(\overline{\alpha})(i)} |\overline{\alpha}_1 \cdots \overline{\alpha}_R \overline{i}_1 \cdots \overline{i}_{\overline{s}}\rangle \tilde{C}_r(\overline{\alpha}_1, \dots, \overline{\alpha}_{\overline{R}}; \overline{i}_1, \dots, \overline{i}_{\overline{s}}), \qquad (C22)$$

so that

$$\overline{C}(\alpha_{1},\ldots,\alpha_{R};i_{1},\ldots,i_{s}) = \sum_{0 \leq r \leq R} \widetilde{C}_{r}(\alpha_{1},\ldots,\alpha_{R};i_{1},\ldots,i_{s})$$

$$= C(\alpha_{1},\ldots,\alpha_{R};i_{1},\ldots,i_{s}) - \sum_{0 \leq r \leq R} \frac{1}{[R|r!(R-r)!]^{1/2}} \sum_{s'=2(R-r)+s}$$

$$\times \sum_{i'_{1}\cdots i'_{s'}} \sum_{P} C(\alpha_{P_{1}},\ldots,\alpha_{P_{1}};i'_{1},\ldots,i'_{s'}) D_{s'}(\alpha_{P_{r+1}},\ldots,\alpha_{P_{R}};i_{1},\ldots,i_{s}|i'_{1},\ldots,i'_{s'}).$$
(C23)

Thus, taking R = 0,

 $0 = \overline{C}(i_1,\ldots,i_N) \equiv C(i_1,\ldots,i_N).$

The remaining follows by induction with the result $C(\alpha_1, \ldots, \alpha_r; i_1, \ldots, i_s) = 0$. Thus the vectors $|\alpha_1 \cdots \alpha_r, i_1 \cdots i_s, f\rangle$ are linearly independent.

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