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Excitation operators associated with antisymmetrized geminal-power states

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Various expressions for antisymmetrized geminal-power (AGP) states are reviewed. With the use of a simple relationship for creation and annihilation operators of BCS (Bardeen, Cooper, and Schrieffer)-type states, such operators are characterized for AGP and GAGP (generalized AGP) schemes. The effect of degeneracy in the first-order reduced density matrix on these operators is displayed.

I. INTRODUCTION

Recent work on the problem of consistency of the random-phase approximation [(RPA) (Refs. 1 and 2)] has lead to the consideration of generalized antisymmetrized geminal-power (GAGP) states[3] as proper vacuums for particle-hole excitations at this level of approximation. Using suitably optimized GAGP states one can construct self-consistent polarization and one-particle-hole propagators that can be associated with a model Hamiltonian.[4,5] This leads to an approximate physical picture that emphasizes the linear-response aspects of the system, the accuracy of which depends on the importance of one-body terms in the exact description.

This approach replaces the uncorrelated Fermi sea, described by independent-particle states (IPS), by a correlated one described by GAGP states as the underlying entity on which one-particle excitations act. The conceptual simplicity of one-particle excitations that either annihilate or create new states from the sea is not lost, as one can define operators that have entirely analogous properties to the conventional particle-hole operators. These operators are described in Secs. III and IV. Such operators have been mentioned previously by Rosina[6] in the context of showing that the second-order reduced density operator of an antisymmetrized geminal-power (AGP) state is uniquely associated with that state. These AGP states are special cases of GAGP states (see Sec. II).

Significantly, these operators are, in fact, not always well defined as the transformation defining them becomes singular when the first-order reduced density operator associated with the GAGP vacuum has eigenvalues that are more than doubly degenerate and a rank greater than N (the number of particles in the system) (Sec. V). This problem was alluded to in Ref. 6 but not studied there. However, we show that in these cases one can replace the normal excitation operators by abnormal ones that are well defined but whose adjoints do not annihilate the vacuum. This has some interesting and profound physical consequences which are discussed elsewhere,[7] and is also reflected in an increased symmetry of the GAGP vacuum.[8]

The AGP states have been extensively considered in the realm of superconductivity[9] where the degeneracy just described plays a key role.[10] They have also been considered as approximate states for molecular systems.[11] The AGP states are particle-number projected Hartree-Fock-Bogolyubov (HFB) states, which are themselves generalized Bardeen-Cooper-Schrieffer states [(BCS) (Refs. 12 and 13)] (BCS states have a fixed pairing assumed between one-particle states while HFB states have a pairing determined by a variational procedure). The HFB states have been comprehensively used in nuclear calculations; see, for instance, Ref. 14 for a recent review. One can associate with such states particle nonconserving quasiparticle excitation operators whose adjoints annihilate the HFB vacuum.[12] The relationship between these various states is reviewed in Sec. II.

The replacement of the IPS (uncorrelated) description of the Fermi sea by the GAGP (correlated) description is a true generalization as the latter includes the former and reduces to it in the absence of interaction. The fact that the correlated excitation operators can be of two types, normal and abnormal—a phenomenon not seen in the uncorrelated case—has profound ramifications which can lead to a particle-conserving theory of superphenomena[7] (unlike BCS theory). The normal excitation operators lead to a model based at a higher level of approximation than the Hartree-Fock (HF) model, for excitations between energy levels in molecular and nuclear (especially light nuclei) systems that maintain particle-number symmetry. This model retains many of the attractive features of the HF approximation that have allowed the ready development of qualitative pictures of physical systems, as the excited states can still be expressed in terms of one-particle operators acting on the ground state.

In this article we extend and rederive some known results that have appeared in less accessible sources (e.g., Ref. 6). However, in contrast to these earlier presentations we wish to emphasize the pertinence of these results for the properties of excited states and excitation spectra.

Notational comments In this text $|v\rangle$ always denotes a normalized vector, v denotes both normalized and unnormalized vectors. $\bar{z}$ signifies the complex conjugate of the complex number z, other notation will be introduced in the course of this article.

II. FORMS OF AN AGP STATE

Pure fermion states are elements of an infinite-dimensional exterior algebra[15] based on a one-particle Hilbert space $\mathscr{H}^1$. The exterior algebra $\mathscr{H}=\wedge(\mathscr{H}^1)$ is itself a Hilbert space and is normally called fermion-Fock space. $\mathscr{H}$ is defined to be the direct sum of $\mathscr{H}^N$, N-particle fermion space, for $N=0,1,\ldots,\infty$, with the inner product defined by the sum of the individual inner products, i.e.,

$$\mathscr{H}=\bigoplus_{N=0}^{\infty}\mathscr{H}^N , \tag{2.1}$$

$$\langle u\,|\,v\rangle=\sum_{N=0}^{\infty}\langle u_N\,|\,v_N\rangle_N\ ,\quad u,v\in\mathscr{H}$$
$$u=\sum_{N=0}^{\infty}u_N\ ,\quad v=\sum_{N=0}^{\infty}v_N\ ,\quad u_N,v_N\in\mathscr{H}^N\ . \tag{2.2}$$

For more details on the construction of $\mathscr{H}$ see, for example, Ref. 16.

The algebraic product in $\mathscr{H}$ is "$\wedge$" the antisymmetrized tensor product defined by

$$v_1\wedge v_2=\tfrac{1}{2}(v_1\otimes v_2-v_2\otimes v_1)$$
$$v_1,v_2\in\mathscr{H}^1\ ; \tag{2.3}$$

$\otimes$ denotes normal tensor product.[15]

An AGP state $\phi_{\rm AGP}$ associated with N particles is a normalized $N/2$th-exterior power of a two-particle fermion state, i.e.,

$$|\,\phi_{\rm AGP}\rangle=|\,g^{N/2}\rangle=c(g)g\wedge\cdots\wedge g=c(g)g^{(N/2)\wedge}\ , \tag{2.4}$$

where $c(g)$ is a normalization factor, $g\in\mathscr{H}^2=\wedge^2\mathscr{H}^1$, and where the product is taken $N/2$ times.

The definition (2.4) together with the term geminal[17] for an element of $\mathscr{H}^2$ justifies the name "antisymmetrized geminal power" describing states of this form.

Any element $g\in\mathscr{H}^2$, can be expressed in canonical form[18] as

$$g=\sum_{i=1}^{s}\zeta_i\,|\,\phi_i\phi_{\bar{i}}\rangle\ , \tag{2.5}$$

where $2s=r=\dim(\mathscr{H}^1)$, $\zeta_i\in c$, $\{\phi_i;1\le i\le r\}$ forms a complete orthonormal basis (conb) of $\mathscr{H}^1$ and $|\,\phi_i\phi_{\bar{i}}\rangle=(1/\sqrt{2})\phi_i\wedge\phi_{i+s}$.

Given any $g\in\mathscr{H}^2$ the form (2.5) can be found by forming the orthogonal projector $|\,g\rangle\langle g\,|$ onto the state g and contracting it to obtain its reduced first-order density operator[19,20] $D^1(g)$, i.e.,

$$D^1(g)=L_2^1(\,|\,g\rangle\langle g\,|\,)\ . \tag{2.6}$$

(For a discussion of the notation L_N^p to describe linear maps : $\mathscr{H}^N\to\mathscr{H}^p$ called contractions see, for example, Refs. 4, 19, and 21.) The projector $|\,g\rangle\langle g\,|$ can equivalently be described as a full two-particle density operator.

The spectrum of $D^1(g)$ is completely discrete, positive, and contains eigenvalues that are at least doubly degenerate (this is due to the antisymmetry of g). Using the spectral theorem we have

$$D^1(g)=\sum_{i=1}^{s}n_i(\,|\,\phi_i\rangle\langle\phi_i\,|+|\,\phi_{i+s}\rangle\langle\phi_{i+s}\,|\,)\ , \tag{2.7}$$

where $\{\phi_i,\phi_{i+s};1\le i\le s\}$ are orthonormal vectors that span the eigenspaces associated with the doubly degenerate eigenvalues $\{n_i;i\le i\le s\}$.

The spin orbitals (elements of $\mathscr{H}^1$ are called such) $\{\phi_i,1\le i\le r\}$ are the canonical ones for g, i.e., g has a Fourier expansion with respect to the conb

$\{ |\phi_i\phi_j\rangle, 1\le i<j\le r\}$ of $\mathscr{H}^2$ given by (2.5). The occupation numbers [i.e., eigenvalues of $D^1(g)$] determine the Fourier coefficients $\{\zeta_i, 1\le j\le s\}$ up to a phase factor, i.e.,

$$\zeta_j = n_j e^{i\theta_j}, \quad i\le j\le s . \tag{2.8}$$

where $0\le\theta_j<2\pi$.

Using the canonical form (2.5) an AGP state can be expressed in configurational form (decomposable elements of $\mathscr{H}^N$ are called n-particle configurations) as

$$|g^{N/2}\rangle = c(g) \sum_{1\le i_1<\cdots<i_{N/2}\le s} \zeta_{i_1}\cdots\zeta_{i_{N/2}} |\phi_{i_1}\phi_{\bar{i}_1}\cdots\phi_{i_{N/2}}\phi_{\bar{i}_{N/2}}\rangle . \tag{2.9}$$

The normalization factor $c(g)$ can be expressed as the inverse square root of the $N/2$th-degree symmetric function $S_{N/2}(\underline{n})$ of the eigenvalues $\{n_i; 1\le j\le s\}$, i.e.,

$$c(g) = S_{N/2}(\underline{n})^{-1/2} , \tag{2.10}$$

$$S_{N/2}(\underline{n}) = \sum_{1\le i_1<\cdots<i_{N/2}\le s} n_{i_1}\cdots n_{i_{N/2}} . \tag{2.11}$$

Another way of writing an AGP utilizes the antisymmetrizer $\mathscr{A}_N$, which is an orthogonal projector

$$\mathscr{A}_N : \otimes^N\mathscr{H}^1 \to \mathscr{A}_N \otimes^N \mathscr{H}^1 \cong \wedge^N\mathscr{H}^1 , \tag{2.12}$$

where $\otimes^N\mathscr{H}^1$ is the full n-fold tensor product of $\mathscr{H}^1$ with itself and $\mathscr{A}_N\otimes^N\mathscr{H}^1$ a subspace of antisymmetric tensors, which is isomorphic to the space $\wedge^N\mathscr{H}^1 = \mathscr{H}^N$. The antisymmetrizer is defined in terms of permutation operators P_σ that form a representation of S_N the symmetric group of degree N, defined by

$$P_\sigma |\phi_{i_1}\cdots\phi_{i_N}\rangle = |\phi_{i_{\sigma(1)}}\cdots\phi_{i_{\sigma(n)}}\rangle , \quad 1\le i_1,\cdots,i_N\le r$$

$$\sigma\in S_N, \quad \sigma:\{1,\ldots,N\}\to\{\sigma(1),\ldots,\sigma(N)\} , \tag{2.13}$$

and σ is a permutation of the integers $\{1,\ldots,N\}$ ($\{|\phi_{i_1}\cdots\phi_{i_N}\rangle; 1\le i_i<\cdots<i_N\le r\}$ forms a conb of $\otimes^N\mathscr{H}^1$ so P_σ is well defined). $\mathscr{A}_N$ is then defined as

$$\mathscr{A}_N = (N!)^{-1}\sum_{\sigma\in S_N}(-1)^{\pi(\sigma)}P_\sigma , \tag{2.14}$$

where $\pi(\sigma)$ is the parity of the permutation σ, i.e., the number of adjacent interchanges necessary to obtain $\{\sigma(1),\ldots,\sigma(N)\}$ from $\{1,\ldots,N\}$. An AGP state can then be expressed as

$$|g^{N/2}\rangle = c(g)\mathscr{A}_N g\otimes\cdots\otimes g , \tag{2.15}$$

where the tensor product is performed $N/2$ times. In the Schrödinger representations this expression translates to a more familiar form, i.e.,

$$\langle x_1\cdots x_N | g^{N/2}\rangle = c(g)\mathscr{A}_N g(x_1x_2)\cdots g(x_{N-1}x_N) , \tag{2.16}$$

where $g(y_1y_2) = \langle y_1y_2 | g\rangle$ and the arguments are space-spin coordinates.

We now introduce the "second quantization" map $a^\dagger(\ ) : \mathscr{H}^1\to B(\mathscr{H})$ for fermions. $B(\mathscr{H})$ is the set of bounded operators acting in $\mathscr{H}$, also called the Fermi-Fock algebra. This c-linear map is defined by

$$a^\dagger(v)|w\rangle = |v\wedge w\rangle , \quad v\in\mathscr{H}^1 , \quad ||v||=1, \forall\ |w\rangle\in\mathscr{H} \tag{2.17}$$

where $|u\rangle$ denotes a normalized vector in the direction of u. This map is easily extendable[21] to an algebraic map:$\mathscr{H}\to B(\mathscr{H})$ and this extension is essentially a normalized left regular representation of the exterior algebra $\mathscr{H}$.

The operators $a^\dagger(v)$ with their adjoints $a(v)$ algebraically generate all of $B(\mathscr{H})$ and satisfy the important canonical anticommutation relationships (CAR):

$$[a^\dagger(v), a^\dagger(w)]_+ = 0 ,$$
$$[a(v), a^\dagger(w)]_+ = \mathrm{Re}\langle v | w\rangle I .$$

If $\{\phi_i, 1\le i\le r\}$ are the canonical spin orbitals of a geminal g then this two-particle antisymmetric function can be written as

$$g = \sum_{i=1}^{s}\zeta_i a^\dagger(\phi_i)a^\dagger(\phi_{\bar{i}})|\phi\rangle = \sum_{i=1}^{s}\zeta_i a_i^\dagger a_{\bar{i}}^\dagger |\phi\rangle = G^\dagger|\phi\rangle , \tag{2.18}$$

where

$$G^\dagger = \sum_{i=1}^{s} \zeta_i a_i^\dagger a_{\bar{i}}^\dagger ,$$

$$a_i^\dagger = a^\dagger(\phi_i), \quad 1 \le i \le r$$

and the vector $|\phi\rangle$ is the normalized vacuum vector that spans $\mathscr{H}^0$. Using this representation of g an AGP state can be expressed as

$$|g^{N/2}\rangle = c(g)(G^\dagger)^{N/2}|\phi\rangle . \tag{2.19}$$

A further form of $|g^{N/2}\rangle$ can be obtained by selecting a reference configuration Φ_B from $\mathscr{H}^N$, then with a normalization constant K

$$|g^{N/2}\rangle = K \sum_{M=0}^{N/2} (M!)^{-2} \left[-\tfrac{1}{4} \sum_{p_1,p_2,h_1,h_2} c_{p_1h_1p_2h_2} b_{p_1}^\dagger b_{h_2} b_{p_2}^\dagger b_{h_2} \right]^M \Phi_B . \tag{2.20}$$

The h_1,h_2 vary over the index set of the occupied spin orbitals in Φ_B and p_1, p_2 over the unoccupied,[22] e.g., if we take the reference configuration to be $|X_1 \cdots X_N\rangle$ then

$$\begin{aligned} b_p^\dagger &= b^\dagger(X_p), \quad N+1 \le p \le r \\ b_h &= b(X_h), \quad 1 \le h \le N . \end{aligned} \tag{2.21}$$

The complex numbers $\{C_{p_1h_1p_2h_2}\}$ are known as correlation coefficients. If the reference configuration is chosen to be a canonical (also called natural) configuration of $|g^{N/2}\rangle$, e.g., $\Phi_B = |\phi_1\phi_{1+s} \cdots \phi_{N/2}\phi_{N/2+s}\rangle$ and the operators $a_p^\dagger$ refer to natural spin orbitals (NSO's) of g, then the expression (2.20) assumes a simpler form (Appendix A), i.e.,

$$\begin{aligned} |g^{N/2}\rangle &= K \sum_{M=0}^{N/2} (M!)^{-2} \\ &\quad \times \left[-\sum_{p,h} C_{php+sh+s} a_p^\dagger a_h a_{p+s}^\dagger a_{h+s} \right]^M \Phi_A . \end{aligned} \tag{2.22}$$

The "correlation" term

$$-\sum_{p,h} C_{php+sh+s} a_p^\dagger a_h a_{p+s}^\dagger a_{h+s}$$

can be factorized as

$$-\sum_{p,h} C_{php+sh+s} a_p^\dagger a_h a_{p+s}^\dagger a_{h+s} = \left[\sum_p \eta_p^P a_p^\dagger a_{p+s}^\dagger \right] \left[\sum_h \eta_h^H a_h a_{h+s} \right] \tag{2.23}$$

so that

$$\underline{C}_{php+sh+s} = (\eta^P \wedge \eta^H)_{pp+shh+s} . \tag{2.24}$$

If the "hole" geminal $G_H = \sum_h \eta_h^H a_h a_{h+s}$ has smaller rank than $N/2$, i.e., the number of nonzero coefficients is strictly less than $N/2$, then (2.22) actually defines a GAGP state Φ_{GAGP}. These are the states of the form

$$|\Phi_{\text{GAGP}}\rangle = |\Phi \wedge g^{N-M/2}\rangle , \tag{2.25}$$

where Φ is an M-particle independent-particle state (IPS) which is strongly orthogonal to $g^{N/2}$, i.e., the NSO's of Φ are orthogonal to those of $g^{N/2}$ or, equivalently, g. The GAGP states can also be formulated in terms of the zero-particle vacuum as

$$|\Phi_{\text{GAGP}}\rangle = \left[\prod_{i=1}^{M} a_i^\dagger \right] (G^\dagger)^{(N-M/2)} |\phi\rangle , \tag{2.26}$$

where

$$G^\dagger = \sum_{i=M+1}^{s} \zeta_i a_i^\dagger a_{i+s}^\dagger . \tag{2.27}$$

One can easily see that GAGP states can be used to describe systems with an *odd* number of fermions by letting M be odd and replacing M by $M \pm 1$ in (2.25) and (2.26).

The relationship between the forms (2.19) and (2.22) is given by

$$\begin{aligned} G^\dagger &= \sum_{1 \le i \le N/2} (\eta_i^H)^{-1} a_i^\dagger a_{i+s}^\dagger + \sum_{N/2+1 \le i \le s} \eta_i^P a_i^\dagger a_{i+s}^\dagger \\ &= \sum_{1 \le i \le s} \zeta_i a_i^\dagger a_{i+s}^\dagger \end{aligned} \tag{2.28}$$

when $\eta_i^H \neq 0$, $1 \le i \le N/2$, and the normalization constant K is given by

$$K = c(g)(n_1 \cdots n_{N/2})^{1/2} = \left[\frac{n_1 \cdots n_{N/2}}{S_{N/2}(\underline{n})} \right]^{1/2} . \tag{2.29}$$

It can be seen from (2.28) that an AGP state becomes a GAGP state when one or more of the coefficients $\{\zeta_i; 1 \le i \le s\}$ becomes infinite. The behavior of the normalization constant K in this case must be examined:

$$\left[\frac{n_1\cdots n_{N/2}}{S_{N/2}(\underline{n})}\right]^{1/2}=\left[1+\sum_{1\le i_1<\cdots<i_{N/2}\le s}{}' n_{i_1}\cdots n_{i_{N/2}}/n_1\cdots n_{N/2}\right]^{-1/2}, \tag{2.30}$$

where the prime in the summation denotes that the term $n_1 \cdots n_{N/2}$ has been omitted. Equation (2.30) is also equal to

$$\left[1+\sum_{1\le i_1<\cdots<i_{N/2-1}\le s}{}' \frac{n_{i_1}\cdots n_{i_{N/2-1}}}{n_2\cdots n_{N/2}}+\frac{1}{n_1}\sum_{1\le i_1<\cdots<i_{N/2-1}\le s}{}' \frac{n_{i_1}\cdots n_{i_{N/2}}}{n_2\cdots n_{N/2}}\right]^{-1/2}. \tag{2.31}$$

(Here the prime denotes the absence of $n_2 \cdots n_{N/2}$.) Letting $n_1 \to \infty$ one finds that Eq. (2.31) yields

$$\left[1+\sum_{1\le i_1\le\cdots<i_{N/2-1}\le s}{}' \frac{n_{i_1}\cdots n_{i_{N/2-1}}}{n_2\cdots n_{N/2}}\right]^{-1/2}=\left[\frac{n_2\cdots n_{N/2}}{S_{N/2-1}(\underline{n})}\right]^{1/2}. \tag{2.32}$$

The behavior of K when $n_i \to \infty$ for one or more $i \in \{1, \ldots, N\}$ thus follows from (2.32).

Yet one more way of obtaining an expression for an AGP state is furnished by HFB-type states ϕ_{HFB}, which do not have a fixed number of particles and are defined by

$$|\phi_{\mathrm{HFB}}\rangle=\beta(g)e^{G^\dagger}|\phi\rangle\ , \tag{2.33}$$

where $\beta(g)$ is a normalization factor and

$$G^\dagger=\sum_{i=1}^{s}\zeta_i a_i^\dagger a_{\bar{i}}^\dagger\ . \tag{2.34}$$

Equation (2.33) is actually a generalization of the states used in superconductivity theory which are there translational invariant i and $\bar{i}$ being associated to modes of opposite momentum and spin.[9,12] In (2.33) any pairing of the degrees of freedom of the system is possible. Equation (2.33) can be expanded to give

$$|\phi_{\mathrm{HFB}}\rangle=\beta(g)\sum_{N=0}^{\infty}(N!)^{-1}g^N\ , \tag{2.35}$$

$$=\beta(g)\sum_{N=0}^{\infty}(N!)^{-1}S_N(\underline{n})^{1/2}|g^N\rangle\ . \tag{2.36}$$

Hence

$$\|\,|\phi_{\mathrm{HFB}}\rangle\|^2=|\beta(g)|^2\sum_{N=0}^{\infty}(N!)^{-2}S_N(\underline{n})\ . \tag{2.37}$$

The series $\sum_{N=0}^{\infty}(N!)^2 S_N(\underline{n})$ can be shown to be convergent,[23] thus leading to a finite value for $\beta(g)$, to give $\|\,|\phi_{\mathrm{HFB}}\rangle\|=1$.

The relationship (2.28) can be further simplified to give the well-known result

$$|\phi_{\mathrm{HFB}}\rangle=\beta(g)\prod_{i=1}^{s}(1+\zeta_i a_i^\dagger a_{\bar{i}}^\dagger)|\phi\rangle\ . \tag{2.38}$$

An AGP state associated with N fermions can be simply formulated in terms of a HFB state as

$$|g^N\rangle=\nu(g)^{-1}P_N|\phi_{\mathrm{HFB}}\rangle\ , \tag{2.39}$$

where P_N is the orthogonal projector onto the subspace $\mathscr{H}^N$ of $\mathscr{H}$ associated with N fermions and

$$\nu(g)=\beta(g)(N/2)!^{-1}S_{N/2}(\underline{n})^{1/2}\ .$$

III. EXCITATION OPERATORS ASSOCIATED WITH AGP STATES

In this section we discuss two linearly independent sets of operators both of which linearly span one-particle operator space, i.e., any one-particle operator can be expressed as linear combinations of them. One of these sets—the set of normal excitation operators—has been displayed previously[6] but the other (abnormal excitation operators), to our knowledge, has not. These sets of operators are important in the construction of self-consistent particle-hole propagators at the random-phase level of approximation.

If we redefine the index $\bar{i}$ to be $-i$, where $1 \le |i| \le s$, it is easy to derive the following relationship from (2.33) (see Appendix B):

$$a_i\,|\,\phi_{\rm HFB}\rangle=\mathrm{sgn}(i)\zeta_i a_{\bar{i}}^\dagger\,|\,\phi_{\rm HFB}\rangle\ ,\quad 1\le|i|\le s\ . \tag{3.1}$$

This implies that

$$\begin{aligned}
a_k^\dagger a_{\bar{i}}P_N\,|\,\phi_{\rm HFB}\rangle&=-\zeta_i P_N a_k^\dagger a_i^\dagger\,|\,\phi_{\rm HFB}\rangle\ ,\\
a_k^\dagger a_i P_N\,|\,\phi_{\rm HFB}\rangle&=\zeta_i P_N a_k^\dagger a_{\bar{i}}^\dagger\,|\,\phi_{\rm HFB}\rangle\ ,\\
a_{\bar{k}}^\dagger a_{\bar{i}}P_N\,|\,\phi_{\rm HFB}\rangle&=-\zeta_i P_N a_{\bar{k}}^\dagger a_i^\dagger\,|\,\phi_{\rm HFB}\rangle\ ,\\
a_{\bar{k}}^\dagger a_i P_N\,|\,\phi_{\rm HFB}\rangle&=\zeta_i P_N a_{\bar{k}}^\dagger a_{\bar{i}}^\dagger\,|\,\phi_{\rm HFB}\rangle\ .
\end{aligned} \tag{3.2}$$

Using the anticommutation relationships and (3.1) on the (rhs) of (3.2) we obtain for $\zeta_k\neq0$

$$a_k^\dagger a_i P_N\,|\,\phi_{\rm HFB}\rangle=\mathrm{sgn}(k)\zeta_i/\zeta_k a_{\bar{i}}^\dagger a_{\bar{k}}P_N\,|\,\phi_{\rm HFB}\rangle\ ,\quad 1\le|i|<|k|\le s \tag{3.3}$$

which gives

$$[\zeta_k a_k^\dagger a_i-\mathrm{sgn}(ik)\zeta_i a_{\bar{i}}^\dagger a_{\bar{k}}]g^{N/2}\rangle=0\ ,\quad 1\le|i|<|k|\le s \tag{3.4}$$

as $|g^{N/2}\rangle$ is colinear with $P_N\,|\,\phi_{\rm HFB}\rangle$. It is thus convenient to define the following operators:

$$q_{ik}=\zeta_k a_k^\dagger a_i-\mathrm{sgn}(ik)\zeta_i a_{\bar{i}}^\dagger a_{\bar{k}}\ ,\quad 1\le|i|<|k|\le s\ . \tag{3.5}$$

We can easily extend the definition (3.5) to the case when $\zeta_k=0$ by noting that

$$\zeta_i a_i^\dagger a_{\bar{k}}\,|\,g^{N/2}\rangle=\zeta_i a_{\bar{i}}^\dagger a_{\bar{k}}\,|\,g^{N/2}\rangle=\zeta_i a_i^\dagger a_k\,|\,g^{N/2}\rangle=\zeta_i a_{\bar{i}}^\dagger a_k\,|\,g^{N/2}\rangle=0\ . \tag{3.6}$$

If $\zeta_i=\zeta_k=0$ we trivially have that

$$a_i^\dagger a_k\,|\,g^{N/2}\rangle=a_k^\dagger a_i\,|\,g^{N/2}\rangle=0\ , \tag{3.7}$$

and it is also easy to see that

$$a_i^\dagger a_{\bar{i}}\,|\,g^{N/2}\rangle=a_{\bar{i}}^\dagger a_i\,|\,g^{N/2}\rangle=(a_i^\dagger a_i-a_{\bar{i}}^\dagger a_{\bar{i}})\,|\,g^{N/2}\rangle=0\ . \tag{3.8}$$

The operators described above all annihilate $|\,g^{N/2}\rangle$, their adjoints produce states that have the following norms (see Appendix C):

$$\|q_{ki}^\dagger\,|\,g^{N/2}\rangle\|=\|q_{\bar{k}\bar{i}}^\dagger\,|\,g^{N/2}\rangle\|=\|q_{k\bar{i}}^\dagger\,|\,g^{N/2}\rangle\|=\|q_{\bar{k}i}^\dagger\,|\,g^{N/2}\rangle\|=S_{N/2}(\underline{n})^{-1/2}(n_i-n_k)\left[\frac{\partial^2 S_{N/2+1}(\underline{n})}{\partial n_i\partial n_k}\right]^{1/2}\ ,\quad 1\le|k|<|i|\le s\ . \tag{3.9}$$

The operators in (3.7) and (3.8) are closed under the adjoint operation, so they and their adjoints annihilate $|\,g^{N/2}\rangle$.

The operator definitions (3.5) and their adjoints can be collected together in matrix form as

$$\begin{bmatrix} q_{ki}^\dagger\\ q_{k\bar{i}}^\dagger\\ q_{\bar{k}i}^\dagger\\ q_{\bar{k}\bar{i}}^\dagger\\ q_{ki}\\ q_{k\bar{i}}\\ q_{\bar{k}i}\\ q_{\bar{k}\bar{i}}\end{bmatrix}=\begin{bmatrix} \bar\zeta_i & & & & & & & -\bar\zeta_k\\ & \bar\zeta_i & & 0 & & & \bar\zeta_k & \\ & & \bar\zeta_i & & & \bar\zeta_k & & \\ & & & \bar\zeta_i & -\bar\zeta_i & & & \\ 0 & & & & & & & 0\\ & & & -\zeta_k & \zeta_i & & & \\ & & \zeta_k & & & \zeta_i & & \\ & \zeta_k & & 0 & & & \zeta_i & \\ -\zeta_k & & & & & & & \zeta_i \end{bmatrix}\begin{bmatrix} a_k^\dagger a_i\\ a_k^\dagger a_{\bar{i}}\\ a_{\bar{k}}^\dagger a_i\\ a_{\bar{k}}^\dagger a_{\bar{i}}\\ a_i^\dagger a_k\\ a_{\bar{i}}^\dagger a_k\\ a_i^\dagger a_{\bar{k}}\\ a_{\bar{i}}^\dagger a_{\bar{k}}\end{bmatrix}\ ,\quad 1\le|k|<|i|\le s\ . \tag{3.10}$$

These transformations define a change of basis for the operator manifold

$$f_2=\mathscr{L}\{a_i^\dagger a_j;1\le|i|,|j|\le s\}, \tag{3.11}$$

where $\mathscr{L}$ denotes linear span, described by

$$(\underline{a}^{\dagger}\underline{a}_{<}\underline{a}^{\dagger}\underline{a}_{>}\underline{\sigma})\rightarrow(\underline{q}^{\dagger}\underline{q}\underline{\sigma}) \ , \tag{3.12}$$

where

$$\{\underline{a}^{\dagger}\underline{a}_{<}\}=\{a_i^{\dagger}a_j;1\leq |i| < |j| \leq s,\zeta_i\neq 0\} \ ,$$

$$\{\underline{a}^{\dagger}\underline{a}_{>}\}=\{(\underline{a}^{\dagger}\underline{a}_{<})^{\dagger}\} \ ,$$

$$\{\underline{\sigma}\}=\{\{a_i^{\dagger}a_i,a_i^{\dagger}a_{\bar{i}},a_{\bar{i}}^{\dagger}a_i,a_{\bar{i}}^{\dagger}a_{\bar{i}};1\leq |i| \leq s\},\{a_i^{\dagger}a_j;1\leq |i|,|j| \leq s,\zeta_i=\zeta_j=0\}\} \ ,$$

the transformation $\underline{T}$ that produces this change of basis can be brought to block diagonal form with 8×8 blocks (3.10) on the diagonal that transform

$$(\underline{a}^{\dagger}\underline{a}_{<}\underline{a}^{\dagger}\underline{a}_{>})\rightarrow(\underline{q}^{\dagger}\underline{q})$$

and a unit matrix that describes the identity $\{\underline{\sigma}\}\rightarrow\{\underline{\sigma}\}$.

The determinant $|\underline{T}|$ of this transformation is easily evaluated as

$$|\underline{T}|=\prod_{1\leq i<k\leq s}(n_i-n_k)^4 \ . \tag{3.13}$$

This transformation is hence nonsingular only when $n_i\neq n_k$, $1\leq i<k\leq s$. If $n_i=n_k$ not only is $\underline{T}$ singular but

$$q_{\bar{k}i}^{\dagger}|g^{N/2}\rangle=q_{\bar{k}\bar{i}}^{\dagger}|g^{N/2}\rangle=q_{ki}^{\dagger}|g^{N/2}\rangle=q_{k\bar{i}}^{\dagger}|g^{N/2}\rangle=0 \ . \tag{3.14}$$

If $n_i=n_k$ we can replace the associated block of $\underline{T}$ by another transformation given by

$$\begin{pmatrix} u_{ki}^{\dagger} \\ u_{k\bar{i}}^{\dagger} \\ u_{\bar{k}i}^{\dagger} \\ u_{\bar{k}\bar{i}}^{\dagger} \\ v_{ki}^{\dagger} \\ v_{k\bar{i}}^{\dagger} \\ v_{\bar{k}i}^{\dagger} \\ v_{\bar{k}\bar{i}}^{\dagger} \end{pmatrix}=\begin{pmatrix} & & & \bar{\zeta}_i & & & & -\zeta_k \\ & & -\bar{\zeta}_i & & & & \zeta_k & \\ & -\bar{\zeta}_i & & & & \zeta_k & & \\ \bar{\zeta}_i & & 0 & & -\zeta_k & & 0 & \\ \bar{\zeta}_k & & & & \zeta_i & & & \\ & \bar{\zeta}_k & & & & \zeta_i & & \\ & & \bar{\zeta}_k & & & & \zeta_i & \\ & & & \bar{\zeta}_k & & & & \zeta_i \end{pmatrix}\begin{pmatrix} a_k^{\dagger}a_i \\ a_k^{\dagger}a_{\bar{i}} \\ a_{\bar{k}}^{\dagger}a_i \\ a_{\bar{k}}^{\dagger}a_{\bar{i}} \\ a_i^{\dagger}a_k \\ a_{\bar{i}}^{\dagger}a_k \\ a_i^{\dagger}a_{\bar{k}} \\ a_{\bar{i}}^{\dagger}a_{\bar{k}} \end{pmatrix} \tag{3.15}$$

with the determinant equal to $(n_i+n_k)^4$. However the adjoints of $\{u_{ki}^{\dagger},u_{\bar{k}i}^{\dagger},u_{\bar{k}i}^{\dagger},u_{\bar{k}\bar{i}}^{\dagger}\}$ do not annihilate $|g^{N/2}\rangle$ nor do the adjoints of $\{v_{ki},v_{k\bar{i}},v_{\bar{k}i},v_{\bar{k}\bar{i}}\}$ produce nonzero states when acting on $|g^{N/2}\rangle$. This result, a consequence of degeneracy amongst n_i's, is a key feature in the excitation spectrum of systems modeled by AGP states.[7]

IV. EXCITATION OPERATORS ASSOCIATED WITH GAGP STATES

The above results can easily be extended to the GAGP case, by using the derivation properly of one particle operators with respect to the product $\wedge$, i.e.,

$$\Omega(a\wedge b)=(\Omega a)\wedge b+a\wedge(\Omega b)\ \forall\, a,b\in\mathscr{H} \ , \tag{4.1}$$

where

$$\Omega=\sum_{1\leq i,j\leq r}\Omega_{ij}a_i^{\dagger}a_j \ . \tag{4.2}$$

Hence

$$q^{\dagger}(\Phi\wedge g^{(N-M)/2})=(q^{\dagger}\Phi)\wedge g^{(N-M)/2}+\Phi\wedge(q^{\dagger}g^{(N-M)/2}) \tag{4.3}$$

and

$$q(\Phi\wedge g^{(N-M)/2})=(q\Phi)\wedge g^{(N-M)/2}+\Phi\wedge(qg^{(N-M)/2}) \ . \tag{4.4}$$

We consider first operators involving spin orbitals in the geminal g, i.e.,

$$q^{\dagger}=q^{\dagger}_{ki},q^{\dagger}_{k\bar{i}},q^{\dagger}_{\bar{k}i},q^{\dagger}_{\bar{k}\bar{i}}$$

and $n_i \neq 0$, $n_k \neq 0$ then $q^{\dagger}\Phi = q\Phi = 0$ and these operators and their adjoints have the same properties as before. If $n_i = n_k \neq 0$ then the corresponding $q^{\dagger},q$ operators can be replaced by the $u^{\dagger},v$ operators in exactly the same way as previously described. When $n_k = 0$ but $n_i \neq 0$ two situations can arise: Either the spin orbitals $\phi_k,\phi_{\bar{k}}$ are totally unoccupied, in which case the operators $q^{\dagger},q$ referring to these subscripts have the same properties as before, or ϕ_k and/or $\phi_{\bar{k}}$ appears in Φ.

(i) ϕ_k and $\phi_{\bar{k}}$ appear in Φ. Then consider $a_l^{\dagger}a_m$, $l=i,\bar{i}$, $m=k,\bar{k}$,

$$\begin{aligned} a_l^{\dagger}a_m(\Phi \wedge g^{(N-M)/2}) &= (a_l^{\dagger}a_m\Phi)\wedge g^{(N-M)/2} + \Phi \wedge (a_l^{\dagger}a_m g^{(N-M)/2}) \\ &= (a_l^{\dagger}a_m\Phi)\wedge g^{(N-M)/2} = 0 \end{aligned} \tag{4.5}$$

while

$$a_m^{\dagger}a_l(\Phi \wedge g^{(N-M)/2}) = (a_m^{\dagger}a_l)\wedge g^{(N-M)/2} + \Phi \wedge (a_m^{\dagger}a_l g^{(N-M)/2}) = 0 \; . \tag{4.6}$$

The first term is zero as ϕ_l does not appear in Φ, while the second term is zero by antisymmetry as ϕ_m appears in every configuration of $a_m^{\dagger}a_l g^{(N-M)/2}$ and is also present in Φ.

(ii) If only ϕ_k appears in Φ then $a_l^{\dagger}a_k$, $l=i,\bar{i}$ have the same properties as in (i) while $a_l^{\dagger}a_{\bar{k}}$ and $a_{\bar{k}}^{\dagger}a_l$ act in the manner of simple particle-hole operators with $a_l^{\dagger}a_{\bar{k}}$ annihilating and $a_{\bar{k}}^{\dagger}a_l$ creating. If $\phi_{\bar{k}}$ appears but ϕ_k does not the roles of k and $\bar{k}$ are just interchanged.

The only remaining case is when the operators refer to spin orbitals that are either occupied or unoccupied in Φ but do not appear at all in $g^{(N-M)/2}$. The properties of these operators are, of course, the same as simple particle-hole operators with respect to an IPS vacuum.

V. EXCITED STATES DERIVED FROM $|g^{N/2}\rangle$

By excited states here we mean the states produced by the operators $\{q^{\dagger}_{kl};k=i,\bar{i};l=j,\bar{j}\}$ acting on $|g^{N/2}\rangle$. First we consider the action of these operators on g, i.e.,

$$q^{\dagger}_{ij}g = (\zeta_j a_i^{\dagger}a_j - \bar{\zeta}_i a_{\bar{j}}^{\dagger}a_{\bar{i}})\sum_{k=1}^{s}\zeta_k\,|\phi_k\phi_{\bar{k}}\rangle = (n_j - n_i)\,|\phi_i\phi_{\bar{j}}\rangle \; , \tag{5.1}$$

$$q^{\dagger}_{i\bar{j}}g = (\bar{\zeta}_j a_i^{\dagger}a_{\bar{j}} + \bar{\zeta}_i a_j^{\dagger}a_{\bar{i}})\sum_{k=1}^{s}\zeta_k\,|\phi_k\phi_{\bar{k}}\rangle = (n_j - n_i)\,|\phi_j\phi_i\rangle \; , \tag{5.2}$$

$$q^{\dagger}_{\bar{i}j}g = (\bar{\zeta}_j a_{\bar{i}}^{\dagger}a_j + \bar{\zeta}_i a_{\bar{j}}^{\dagger}a_i)\sum_{k=1}^{s}\zeta_k\,|\phi_k\phi_{\bar{k}}\rangle = (n_j - n_i)\,|\phi_{\bar{i}}\phi_{\bar{j}}\rangle \; , \tag{5.3}$$

$$q^{\dagger}_{\bar{i}\bar{j}}g = (\bar{\zeta}_j a_{\bar{i}}^{\dagger}a_{\bar{j}} - \bar{\zeta}_i a_j^{\dagger}a_i)\sum_{k=1}^{s}\zeta_k\,|\phi_k\phi_{\bar{k}}\rangle = (n_j - n_i)\,|\phi_j\phi_{\bar{i}}\rangle \; , \tag{5.4}$$

when $n_i = n_j$ we can replace the $q^{\dagger}$'s by $u^{\dagger}$'s as before and one obtains that

$$\begin{aligned} u^{\dagger}_{ij}g &= (n_j + n_i)\,|\phi_i\phi_{\bar{j}}\rangle \; , \\ u^{\dagger}_{i\bar{j}}g &= (n_j + n_i)\,|\phi_j\phi_i\rangle \; , \\ u^{\dagger}_{\bar{i}j}g &= (n_j + n_i)\,|\phi_{\bar{i}}\phi_{\bar{j}}\rangle \; , \\ u^{\dagger}_{\bar{i}\bar{j}}g &= (n_j + n_i)\,|\phi_i\phi_{\bar{j}}\rangle \; , \end{aligned} \tag{5.5}$$

which are the same set (up to norms) of two-particle states as in (5.1)–(5.4).

We call the excitation operators $\{q^{\dagger}_{kl};k=i,\bar{i};l=j,\bar{j}\}$ *normal* and $\{u^{\dagger}_{kl};k=i,\bar{i};l=j,\bar{j}\}$ *abnormal*. This distinction is of crucial importance in our discussion of sum rules, ground-state degeneracy, and the existence of the effective Hamiltonian associated with a self-consistent particle-hole propagator (SCIPHP).[7]

Using the relationship (4.1) the effect of $q^{\dagger}$ (or $u^{\dagger}$) operators on $g^{N/2}$ is easily obtained:

$$q^{\dagger}_{ij}g^{N/2} = q^{\dagger}_{ij}g \wedge \cdots \wedge g = \frac{N}{2}(q^{\dagger}_{ij}g)\wedge g^{N/2-1} \; , \tag{5.6}$$

where the product is taken $N/2$ times (using the commutativity of two-particle functions with respect to $\wedge$)

$$q_{ij}^{\dagger}g^{N/2}=\frac{N}{2}(n_j-n_i)\,|\,\phi_i\phi_{\bar{j}}\rangle\wedge g^{N/2-1}\,. \quad (5.7)$$

Similarly,

$$q_{i\bar{j}}^{\dagger}g^{N/2}=\frac{N}{2}(n_j-n_i)\,|\,\phi_j\phi_i\rangle\wedge g^{N/2-1}\,,$$

$$q_{\bar{i}\bar{j}}^{\dagger}g^{N/2}=\frac{N}{2}(n_j-n_i)\,|\,\phi_{\bar{i}}\phi_{\bar{j}}\rangle\wedge g^{N/2-1}\,, \quad (5.8)$$

$$q_{\bar{i}j}^{\dagger}g^{N/2}=\frac{N}{2}(n_j-n_i)\,|\,\phi_j\phi_{\bar{i}}\rangle\wedge g^{N/2-1}\,.$$

As the spin orbitals $\{\phi_i,\phi_{\bar{i}},\phi_j,\phi_{\bar{j}}\}$ appear in g, (5.7) and (5.8) can be reexpressed in GAGP form, e.g.,

$$q_{ij}^{\dagger}g^{N/2}=\frac{N}{2}(n_j-n_i)\,|\,\phi_i\phi_{\bar{j}}\rangle\wedge\tilde{g}^{N/2-1}\,,$$

where

$$\tilde{g}=\sum_{k\neq i,j}^{S}\zeta_k\,|\,\phi_k\phi_{\bar{k}}\rangle\,. \quad (5.9)$$

The $u^{\dagger}$ operators give rise to the same excited states except that they are multiplied by a factor (n_j+n_i) instead of (n_j-n_i).

The excited states obtained from a GAGP state are easily analyzed in the same way.

"Doubly" excited states can be of the following type:

$$\left.\begin{array}{l} q_{kl}^{\dagger}q_{ij}^{\dagger}g^{N/2}\,, \\ q_{kl}q_{ij}^{\dagger}g^{N/2}\,. \end{array}\right\} k=\bar{k}_1,k_1,\;\; l=\bar{l}_1,l_1,\;\; i=\bar{i}_1,i_1,\;\; j=\bar{j}_1,j_1 \quad (5.10)$$

After some algebra these states can be shown to be of the form (except for constant factors)

$$(\bar{\zeta}_j\,|\,\phi_i\phi_{\bar{i}}\rangle-\bar{\zeta}_i\,|\,\phi_j\phi_{\bar{j}}\rangle)\wedge g^{N/2-1}+|\,\phi_i\phi_{\bar{i}}\phi_j\phi_{\bar{j}}\rangle\wedge g^{N/2-2}\,, \quad (5.11)$$

$$|\,\phi_k\phi_l\rangle\wedge g^{N/2-1}+|\,\phi_i\phi_{\bar{i}}\phi_k\phi_l\rangle\wedge g^{N/2-2},\;\; k\neq l,\bar{l},i,\bar{i},\;\; l\neq i,\bar{i} \quad (5.12)$$

$$|\,\phi_i\phi_j\phi_k\phi_l\rangle\wedge g^{N/2-2,}\;\; i\neq j,\bar{j},k,\bar{k},l,\bar{l},\;\; j=k,\bar{k},l,\bar{l},\;\; k\neq l,\bar{l}$$

and

$$(\zeta_i\,|\,\phi_i\phi_{\bar{i}}\rangle-\zeta_j\,|\,\phi_j\phi_{\bar{j}}\rangle)\wedge g^{N/2-2},\;\; |\,kl\rangle\wedge g^{N/2-1,}\;\; k\neq l,\bar{l}\,. \quad (5.13)$$

VI. DISCUSSION

We have shown that one can associate dressed annihilators and creators with GAGP states in analogy with IPS and associated particle-hole and hole-particle operators. Furthermore, the excited states produced by these creators also have GAGP form. The creators depend explicitly on the canonical expansion coefficients of the geminal, while the norms of the excited states produced by each of these creators are proportional to differences of the occupation numbers of the one matrix of the geminal. Degeneracies of this matrix have two consequences: the ordinarily valid prescription for constructing excitation operators has to be changed and the new one leads to creators whose adjoints are not annihilators. Significant ramifications of this are seen in the linear-response properties of the GAGP model, as well as increased degeneracy of the vacuum and hence implied symmetry breaking. We discuss this elsewhere.[7,24]

APPENDIX A

The form of a state consistent with one-particle excitation and annihilation operators is

$$\Psi=\sum_{m=0}^{N}(m!)^{-2}\times\left[-\sum_{\substack{1\leq h_1<h_2\leq N\\ N+1\leq p_1<p_2\leq r}}C_{p_1h_1p_2h_2}b_{p_1}^{\dagger}b_{h_1}b_{p_2}^{\dagger}b_{h_2}\right]^m\Phi_B\,, \quad (A1)$$

where

(i) $\Phi_B=|\,\chi_1\cdots\chi_N\rangle$,

(ii) $C_{p_1h_1p_2h_2}=\zeta_{p_1p_2}^{P}\zeta_{h_1h_2}^{H}$,

(iii) $\zeta_{p_1p_2}^{P}=-\zeta_{p_2p_1}^{P},\;\;\zeta_{h_1h_2}^{H}=-\zeta_{h_2h_1}^{H}$.

Thus

$$-\sum_{1\le h_1<h_2\le N;N+1\le p_1<p_2\le r} C_{p_1h_2p_2h_2}b^\dagger_{p_1}b_{h_1}b^\dagger_{p_2}b_{h_2} = G^\dagger_P G_H \ , \quad (A2)$$

where

$$G^\dagger_P = \sum_{N+1\le p_1<p_2\le r} \zeta^P_{p_1p_2}b^\dagger_{p_1}b^\dagger_{p_2}$$

and

$$G_H = \sum_{1\le h_1<h_2\le N} \zeta^H_{h_1h_2}b_{h_1}b_{h_2} \ .$$

By considering the antisymmetric states

$$G^\dagger_P\,|\,\phi\rangle = \tfrac{1}{2}\sum_{N+1\le p_1,p_2\le r} \zeta^P_{p_1p_2}\,|\,\chi_{p_1}\chi_{p_2}\rangle \quad (A3)$$

and

$$G^\dagger_H\,|\,\phi\rangle = \tfrac{1}{2}\sum_{1\le h_1,h_2\le N} \bar{\zeta}^H_{h_1,h_2}\,|\,\chi_{h_1}\chi_{h_2}\rangle \quad (A4)$$

we can find unitary transformations

$$U:\mathscr{H}^1_h \to \mathscr{H}^1_h \ , \quad (A5)$$

where $\mathscr{H}^1_h$ is the Hilbert space spanned by the occupied spin orbitals and

$$V:\mathscr{H}^1_p \to \mathscr{H}^1_p \ , \quad (A6)$$

where $\mathscr{H}^1_p$ is the Hilbert space spanned by the unoccupied spin orbitals such that

$$G^\dagger_p\,|\,\phi\rangle = \tfrac{1}{2}\sum_{N+1\le p_1,p_2\le r} \eta^P_{p_1p_2}\,|\,\phi_{p_1}\phi_{p_2}\rangle = \sum_{N+1\le p\le[r-N]/2} \eta^P_{pp+\nu}\,|\,\phi_p\phi_{p+\nu}\rangle \ , \quad (A7)$$

where

$$\nu=[r-N]/2$$

and

$$[K]=\begin{cases} K & \text{if } K \text{ is even} \\ K-1 & \text{if } K \text{ is odd} \end{cases}$$

$$G^\dagger_h\,|\,\phi\rangle = -\tfrac{1}{2}\sum_{1\le h_1,h_2\le N} \bar{\eta}_{h_1h_2}\,|\,\phi_{h_1}\phi_{h_2}\rangle = -\sum_{1\le h\le[N]/2} \bar{\eta}^H_{hh+\nu}\,|\,\phi_h\phi_{h+\nu}\rangle \ , \quad (A8)$$

where in this case $\nu=[N]/2$. (It should be noted that $r=2s$, i.e., is always even due to the spin of electrons.) The change of basis (A5) and (A6) can be written as

$$\underline{\phi}_h = \underline{\chi}_h\underline{U} \ , \quad (A9)$$

$$\underline{\phi}_p = \underline{\chi}_p\underline{V} \ . \quad (A10)$$

(We have assumed that the set $\{\phi_i; 1\le i\le r\}$ is a conb for $\mathscr{H}^1$.) Hence from Eqs. (A3) and (A7) and Eqs. (A4) and (A8) we have

$$\tfrac{1}{2}\sum_{N+1\le p_1,p_2\le r} \zeta^P_{p_1p_2}\,|\,\chi_{p_1}\chi_{p_2}\rangle = \tfrac{1}{2}\sum_{\substack{N+1\le p_1,p_2\le r\\ N+1\le p_3,p_4\le r}} \eta^P_{p_3p_4}V_{p_1p_3}V_{p_2p_4}\,|\,\chi_{p_1}\chi_{p_2}\rangle \ , \quad (A11)$$

$$-\tfrac{1}{2}\sum_{N+1\le p_1,p_2\le r} |\,\chi_{h_1}\chi_{h_2}\rangle = -\tfrac{1}{2}\sum_{\substack{1\le h_1,h_2\le N\\ 1\le h_3,h_4\le N}} \bar{\eta}^H_{h_3h_4}U_{h_1h_3}U_{h_2h_4}\,|\,\chi_{h_1}\chi_{h_2}\rangle \ , \quad (A12)$$

so that

$$\underline{\bar{\zeta}}^P = \underline{V}\,\underline{\eta}^P\underline{V}^t \quad (A13)$$

and

$$\underline{\bar{\zeta}}^H = \underline{U}\,\underline{\bar{\eta}}^H\underline{U}^t \ . \quad (A14)$$

As

$$\underline{V}^\dagger\underline{V} = \underline{V}\underline{V}^\dagger = I_{r-N} \quad (A15)$$

and

$$\underline{U}^\dagger\underline{U} = \underline{U}\underline{U}^\dagger = I_N \ . \quad (A16)$$

We obtain from (A13) and (A14) that

$$\underline{V}^\dagger\underline{\zeta}^P\underline{\bar{V}} = \underline{\eta}^P \quad (A17)$$

and

$$\underline{U}^\dagger\underline{\bar{\zeta}}^H\underline{\bar{U}} = \underline{\bar{\eta}}^H \leftrightarrow \underline{U}^t\underline{\zeta}^H\underline{U} = \underline{\eta}^H \quad (A18)$$

and the matrices $\underline{\eta}^P, \underline{\eta}^H$ have the following structure:

$$\underline{\eta}^P_{p_1p_2} = \underline{\eta}^P_{p_1p_1+\nu}\delta_{p_1p_2-\nu}, \quad \nu=[r-N]/2$$
$$\underline{\eta}^P_{p_1p_2} = -\underline{\eta}^P_{p_2p_1}, \quad N+1\le p_1\le p_2\le r \quad (A19)$$

$$\underline{\eta}^H_{h_1h_2} = \underline{\eta}^H_{h_1h_1+\nu}\delta_{h_1h_2-\nu}, \quad \nu=[N]/2$$
$$\underline{\eta}^H_{h_1h_2} = -\eta^H_{h_2h_1}, \quad 1\le h_1\le h_2\le N \ . \quad (A20)$$

The operators U and V, that have matrix representation $\bar{U}$ and $\underline{V}$ with respect to the bases

$\{\chi_h; 1 \le h \le N\}$ and $\{\chi_p; N+1 \le p \le r\}$ of $\mathscr{H}_h^1$ and $\mathscr{H}_p^1$ have representations over Fock space given by

$$U = \exp\left[i \sum_{1 \le h_1, h_2 \le N} \lambda_{h_1 h_2} b_{n_1}^\dagger b_{h_2}\right], \quad (A21)$$

$$V = \exp\left[i \sum_{N+1 \le p_1, p_2 \le r} \lambda_{p_1 p_2} b_{p_1}^\dagger b_{p_2}\right], \quad (A22)$$

where

$$\underline{U} = e^{i\lambda^P}, \quad \underline{V} = e^{i\lambda^H},$$
$$\lambda_{p_1 p_2} = \lambda_{p_1 p_2}^P, \quad \lambda_{h_1 h_2} = \lambda_{h_1 h_2}^H, \quad (A23)$$

and we have used U and V to denote the operators defined both over $\mathscr{H}_h^1, \mathscr{H}_p^1$, and Fock space $\mathscr{H}$.

Letting $\{a_i^\dagger; 1 \le i \le r\}$ be the field operators associated with the basis $\{\phi_i, 1 \le i \le r\}$ we can see that

$$a_h^\dagger = U b_n^\dagger U^\dagger, \quad 1 \le h \le N \quad (A24)$$

and

$$a_p^\dagger = V b_p^\dagger V^\dagger, \quad N+1 \le p \le r . \quad (A25)$$

As

$$U b_n^\dagger U^\dagger = \sum_{1 \le h' \le N} b_{h'}^\dagger \underline{U}_{h'h} \quad (A26)$$

and

$$V b_p^\dagger V^\dagger = \sum_{N+1 \le p' \le r} b_{p'}^\dagger \underline{V}_{p'p} \quad (A27)$$

we can see that

$$G_P^\dagger = \tfrac{1}{2} \sum_{N+1 \le p_1, p_2 \le r} \zeta_{p_1 p_2}^P b_{p_1}^\dagger b_{p_2}^\dagger$$
$$= \tfrac{1}{2} \sum_{N+1 \le p_1, p_2 \le r} \eta_{p_1 p_2}^P a_{p_1}^\dagger a_{p_2}^\dagger , \quad (A28)$$

and

$$G_H^\dagger = -\tfrac{1}{2} \sum_{1 \le h_1, h_2 \le N} \bar{\zeta}_{h_1 h_2}^H b_{h_1}^\dagger b_{h_2}^\dagger$$
$$= -\tfrac{1}{2} \sum_{1 \le h_1, h_2 \le N} \bar{\eta}_{h_1 h_2}^H a_{h_1}^\dagger a_{h_2}^\dagger , \quad (A29)$$

$$G_H = \tfrac{1}{2} \sum_{1 \le h_1, h_2 \le N} \zeta_{h_1 h_2}^H b_{h_1} b_{h_2}$$
$$= \tfrac{1}{2} \sum_{1 \le h_1, h_2 \le N} \eta_{h_1 h_2}^H a_{h_1} a_{h_2} . \quad (A30)$$

Noting that as U is a unitary map $: \mathscr{H}_h \to \mathscr{H}_h$

$$\Phi_A = U\Phi_B = |(U\chi_1) \wedge \cdots \wedge (U\chi_N)\rangle$$
$$= e^{i\alpha} |\chi_1 \wedge \cdots \wedge \chi_N\rangle$$
$$\equiv \Phi_B \text{ as a state, } \alpha \in [0, 2\pi] . \quad (A31)$$

The state Ψ can be written in a rather simple form as

$$\Psi = \sum_{m=0}^{[N]/2} (m!)^{-2} (G_P^\dagger G_H)^m \Phi_A = \sum_{m=0}^{[N]/2} (m!)^{-2} \left[\sum_{\substack{n+1 \le p \le [r-N]/2 \\ 1 \le h \le [N]/2}} \eta_p^P \eta_h^H a_p^\dagger a_{\bar{p}}^\dagger a_h a_{\bar{h}}\right]^m \Phi_A , \quad (A32)$$

where

$$\bar{p} = p + [r-N]/2$$

and

$$\bar{h} = h + [N]/2 .$$

If the number of nonzero η_h^H is less than $[N]/2$ the spin orbitals corresponding to the zero coefficient will be in all the configurations produced from Φ_A. So Ψ will have the form

$$\Psi = |\Phi \wedge g^{M/2}\rangle , \quad (A33)$$

where

$$\Phi = |\phi_1 \cdots \phi_v\rangle$$

and

$$v = ([N] - M)/2; \quad M = 2X$$

where X represents the number of nonzero coefficients. The spin orbitals $\{\phi_i; 1 \le i \le r\}$ are easily seen to be the NSO's of Ψ as the configurations produced in (A32) are at least different in two positions from each other.

APPENDIX B

We have the following:

$$a_{\bar{k}} \prod_{i=1}^{s} (1 + \zeta_i a_i^\dagger a_{\bar{i}}^\dagger) |\phi\rangle = \prod_{i=1, i \ne k}^{s} (1 + \zeta_i a_i^\dagger a_{\bar{i}}^\dagger) a_{\bar{k}} \zeta_k a_k^\dagger a_{\bar{k}} |\phi\rangle$$

$$= -\prod_{i=1,i\neq k}^{s}(1+\zeta_i a_i^\dagger a_{\bar{i}}^\dagger)\zeta_k a_{\bar{k}}^\dagger a_{\bar{k}} a_{\bar{k}}^\dagger |\phi\rangle$$

$$= -\prod_{i=1,i\neq k}^{s}(1+\zeta_i a_i^\dagger a_{\bar{i}}^\dagger)\zeta_{kk}^\dagger(1-a_{\bar{k}}^\dagger a_{\bar{k}})|\phi\rangle$$

$$= -\prod_{i=1,i\neq k}^{s}(1+\zeta_i a_i^\dagger a_{\bar{i}}^\dagger)\zeta_k a_k^\dagger |\phi\rangle$$

$$= \sum_{i=1,i\neq k}^{s}(1+\zeta_i a_i^\dagger a_{\bar{i}}^\dagger)\zeta_k a_k^\dagger(1+\zeta_k a_k^\dagger a_{\bar{k}}^\dagger)|\phi\rangle$$

$$= -\zeta_k a_k^\dagger \prod_{i=1}^{s}(1+\zeta_i a_i^\dagger a_{\bar{i}}^\dagger)|\phi\rangle ,$$

(as $[a_i^\dagger a_{\bar{i}}^\dagger, a_j^\dagger a_{\bar{j}}^\dagger]_- = 0$ and $[a_{\bar{k}}, a_i^\dagger a_{\bar{i}}^\dagger]_- = 0$ if $i\neq k$) similarly,

$$a_k\prod_{i=1}^{s}(1+\zeta_i a_i^\dagger a_{\bar{i}}^\dagger)|\phi\rangle = \prod_{i=1,i\neq k}^{s}(1+\zeta_i a_i^\dagger a_{\bar{i}}^\dagger)a_k\zeta_k a_k^\dagger a_{\bar{k}}^\dagger |\phi\rangle$$

$$= \prod_{i=1,i\neq k}^{s}(1+\zeta_i a_i^\dagger a_{\bar{i}}^\dagger)\zeta_k a_{\bar{k}}^\dagger |\phi\rangle$$

$$= \prod_{i=1,i\neq k}^{s}(1+\zeta_i a_i^\dagger a_{\bar{i}}^\dagger)\zeta_k a_{\bar{k}}^\dagger(1+\zeta_k a_k^\dagger a_{\bar{k}}^\dagger)|\phi\rangle$$

$$= \zeta_k a_{\bar{k}}^\dagger \prod_{i=1}^{s}(1+\zeta_i a_i^\dagger a_{\bar{i}}^\dagger)|\phi\rangle .$$

APPENDIX C

We have the following:

$$\left.\begin{aligned} q_{i\bar{j}} &= \zeta_j a_{\bar{j}}^\dagger a_i + \zeta_i a_{\bar{i}}^\dagger a_j , \\ q_{\bar{i}j} &= \zeta_j a_j^\dagger a_{\bar{i}} - \zeta_j a_i^\dagger a_{\bar{j}} , \end{aligned}\right\} 1 \le i < j \le s \tag{C1}$$

$$q_{ij} = \zeta_j a_{\bar{j}}^\dagger a_{\bar{i}} - \zeta_i a_i^\dagger a_j, \quad 1 \le i,j \le s . \tag{C2}$$

There are six types of overlap integrals between the excited states to be considered. As $q_{\bar{i}\bar{j}} = q_{ji}$, $1 \le i < j \le s$ we need only consider (C1) and (C2) as follows.

Type 1:

$$\langle g^{N/2} | q_{i\bar{j}} q_{k\bar{l}}^\dagger g^{N/2}\rangle$$

$$= \langle g^{N/2} | (\zeta_j a_{\bar{j}}^\dagger a_i + \zeta_i a_{\bar{i}}^\dagger a_j)(\zeta_k a_{\bar{k}}^\dagger a_l + \zeta_l a_{\bar{l}}^\dagger a_k) g^{N/2}\rangle , \tag{C3}$$

$$\begin{aligned} &= \bar{\zeta}_k\zeta_j D^1(g^{N/2})_{\bar{j}\bar{k}}\delta_{il} + \bar{\zeta}_l\zeta_j D^1(g^{N/2})_{\bar{j}\bar{l}}\delta_{ik} + \bar{\zeta}_k\zeta_i D^1(g^{N/2})_{\bar{i}\bar{k}}\delta_{jl} + \bar{\zeta}_l\zeta_i D^1(g^{N/2})_{\bar{i}\bar{l}}\delta_{jk} \\ &\quad - \bar{\zeta}_k\zeta_j D^2(g^{N/2})_{\bar{j}l\bar{k}i} - \bar{\zeta}_l\zeta_j D^2(g^{N/2})_{\bar{j}k\bar{l}i} - \bar{\zeta}_k\zeta_i D^2(g^{N/2})_{\bar{i}l\bar{k}j} - \bar{\zeta}_l\zeta_i D^2(g^{N/2})_{\bar{i}k\bar{l}j} , \end{aligned} \tag{C4}$$

$$\begin{aligned} &= (\delta_{kj}\delta_{il} + \delta_{jl}\delta_{ik})[(\eta_j\eta_{1j} + \eta_i\eta_{1i}) - \bar{\zeta}_k\zeta_j D^2(g^{N/2})_{l\bar{j}i\bar{k}} - \bar{\zeta}_l\zeta_j D^2(g^{N/2})_{k\bar{j}i\bar{l}} \\ &\qquad - \bar{\zeta}_k\zeta_i D^2(g^{N/2})_{l\bar{i}j\bar{k}} - \bar{\zeta}_l\zeta_i D^2(g^{N/2})_{k\bar{i}j\bar{l}}] , \end{aligned} \tag{C5}$$

where η_{1i}'s are eigenvalues of $D^1(g^{N/2})$. [The first-order reduced density matrix of the AGP state $|g^{N/2}\rangle$, and $D^2(g^{N/2})$ is the corresponding second-order one.] If $k=j$ and $i=l$ but $k\neq i$ ($\rightarrow j\neq l$), then (C5) is equal to

$$\eta_j\eta_{1j}+\eta_i\eta_{1i}-\eta_j d^2(g^{N/2})_{i\bar{j}i\bar{j}}-\bar{\zeta}_i\zeta_j D^2(g^{N/2})_{j\bar{j}i\bar{i}}-\bar{\zeta}_j\zeta_i D^2(g^{N/2})_{i\bar{i}j\bar{j}}-\eta_i D^2(g^{N/2})_{j\bar{i}j\bar{i}}\ , \tag{C6}$$

$$=\eta_j^2 S_{N/2}^{-1}\frac{\partial S_{N/2}}{\partial\eta_j}+\eta_i^2 S_{N/2}^{-1}\frac{\partial S_{N/2}}{\partial\eta_i}-\eta_j^2\eta_i S_{N/2}^{-1}\frac{\partial^2 S_{N/2}}{\partial\eta_i\partial\eta_j}-\eta_i\eta_j S_{N/2}^{-1}\frac{\partial^2 S_{N/2}+1}{\partial\eta_i\partial\eta_j}-\eta_i\eta_j S_{N/2}^{-1}\frac{\partial^2 S_{N/2}+1}{\partial\eta_i\partial\eta_j}$$
$$-\eta_i^2\eta_j S_{N/2}^{-1}\frac{\partial^2 S_{N/2}}{\partial\eta_i\partial\eta_j}\ , \tag{C7}$$

$$=S_{N/2}^{-1}\left[\eta_j^2\frac{\partial S_{N/2}}{\partial\eta_j}+\eta_i^2\frac{\partial S_{N/2}}{\partial\eta_i}-\eta_i\eta_j\left[\eta_j\frac{\partial^2 S_{N/2}}{\partial\eta_i\partial\eta_j}+\eta_i\frac{\partial^2 S_{N/2}}{\partial\eta_i\partial\eta_j}+2\frac{\partial^2 S_{N/2}+1}{\partial\eta_i\partial\eta_j}\right]\right]\ . \tag{C8}$$

Now

$$\frac{\partial S_{N/2}}{\partial\eta_j}=\sum_{1\le j_1<\cdots<i_{N/2-1}\le s}^{i}\eta_{i_1}\cdots\eta_{i_{N/2-1}}\ , \tag{C9}$$

$$\frac{\partial S_{N/2}}{\partial\eta_i}=\sum_{1\le i_1<\cdots<i_{N/2-1}\le s}^{i}\eta_{i_1}\cdots\eta_{i_{N/2-1}}\ , \tag{C10}$$

$$\frac{\partial^2 S_{N/2}}{\partial\eta_i\partial\eta_j}=\sum_{1\le i_1<\cdots<i_{N/2-2}\le s}^{ij}\eta_{i_1}\cdots\eta_{i_{N/2-2}}\ , \tag{C11}$$

$$\frac{\partial^2 S_{N/2+1}}{\partial\eta_i\partial\eta_j}=\sum_{1\le i_1<\cdots<i_{N/2-1}\le s}^{ij}\eta_{i_1}\cdots\eta_{i_{N/2-1}}\ , \tag{C12}$$

where $\sum^{kl\cdots}$ denotes the omission of the $k,l,\ldots$ terms from the sum. Therefore (C8) gives

$$S_{N/2}^{-1}\left[\eta_j^2\sum_{1\le j_1<\cdots<i_{N/2-1}\le s}^{i}\eta_{i_1}\cdots\eta_{i_{N/2-1}}+\eta_i^2\sum_{i\le i_1<\cdots<i_{N/2-1}\le s}^{i}\eta_{i_1}\cdots\eta_{i_{N/2-1}}\right.$$
$$-\eta_i\eta_j\left[\eta_j\sum_{1\le i_1<\cdots<i_{N/2-2}\le s}^{ij}\eta_{i_1}\cdots\eta_{i_{N/2-2}}+\eta_i\sum_{1\le i_1<\cdots<i_{N/2-2}\le s}^{ij}\eta_{i_1}\cdots\eta_{i_{N/2-2}}\right.$$
$$\left.\left.+2\sum_{1\le i_1<\cdots<i_{N/2-1}\le s}\eta_{i_1}\cdots\eta_{i_{N/2-1}}\right]\right]\ , \tag{C13}$$

$$=S_{N/2}^{-1}\left[\eta_j^2\eta_i\sum_{1\le i_1<\cdots<i_{N/2-2}\le s}^{ij}\eta_{i_1}\cdots\eta_{i_{N/2-2}}+\eta_j^2\sum_{1\le i_1<\cdots<i_{N/2-1}\le s}^{j}\eta_{i_1}\cdots\eta_{i_{N/2-1}}\right.$$
$$+\eta_i^2\eta_j\sum_{1\le i_1<\cdots<i_{N/2-2}\le s}^{ij}\eta_{i_1}\cdots\eta_{i_{N/2-2}}+\eta_i^2\sum_{1\le i_1<\cdots<i_{N/2-1}\le s}^{i}\eta_{i_1}\cdots\eta_{i_{N/2-1}}$$
$$\left.-\eta_i\eta_j(\eta_i+\eta_j)\sum_{1\le i_1<\cdots<i_{N/2-1}\le s}^{ij}\eta_{i_1}\cdots\eta_{i_{N/2-1}}-2\eta_i\eta_j\sum_{1\le i_1<\cdots<i_{N/2-2}\le s}^{ij}\eta_{i_1}\cdots\eta_{i_{N/2-2}}\right]\ , \tag{C14}$$

$$=S_{N/2}^{-1}(\eta_i-\eta_j)^2\sum_{1\le i_1<\cdots<i_{N/2-1}\le s}^{ij}\eta_{i_1}\cdots\eta_{i_{N/2-1}}\ . \tag{C15}$$

If $k=i$ and $l=j$ but $k\neq j$ ($\rightarrow i\neq l$), Eq. (C5) equals

$$\eta_i\eta_{1i}+\eta_j\eta_{1j}=\bar{\zeta}_i\zeta_j D^2(g^{N/2})_{j\bar{j}i\bar{i}}-\eta_j D^2(g^{N/2})_{i\bar{j}i\bar{j}}-\eta_i D^2(g^{N/2})_{j\bar{i}j\bar{i}}-\bar{\zeta}_j\zeta_i D^2(g^{N/2})_{i\bar{i}j\bar{j}}\ , \tag{C16}$$

and we can see that Eq. (C16) equals Eq. (C6). Hence

$$\langle q_{ij}^{\dagger} g^{N/2} | q_{k\bar{l}}^{\dagger} g^{N/2} \rangle = (\delta_{ik}\delta_{lj} + \delta_{il}\delta_{kj}) S_{N/2}^{-1} (\eta_i - \eta_j)^2 \sum_{1 \le i_1 < \cdots < i_{N/2-1} \le s}^{ij} \eta_{i_1} \cdots \eta_{i_{N/2-1}} . \tag{C17}$$

Type 2:

$$\langle g^{N/2} | q_{i\bar{j}} q_{\bar{k}l}^{\dagger} g^{N/2} \rangle$$

$$= \langle g^{N/2} | (\zeta_j a_{\bar{j}}^{\dagger} a_i + \zeta_i a_{\bar{i}}^{\dagger} a_j)(\zeta_k a_k^{\dagger} a_{\bar{l}} + \zeta_l a_l^{\dagger} a_{\bar{k}})^{\dagger} g^{N/2} \rangle \tag{C18}$$

$$= \langle g^{N/2} | (-\zeta_j \bar{\zeta}_k a_{\bar{j}}^{\dagger} a_{\bar{l}}^{\dagger} a_i a_k - \zeta_j \bar{\zeta}_l a_{\bar{j}}^{\dagger} a_{\bar{k}}^{\dagger} a_i a_l - \zeta_i \bar{\zeta}_k a_{\bar{i}}^{\dagger} a_{\bar{l}}^{\dagger} a_j a_k - \zeta_i \bar{\zeta}_l a_{\bar{i}}^{\dagger} a_{\bar{k}}^{\dagger} a_j a_l) g^{N/2} \rangle . \tag{C19}$$

Equation (C19) equals zero, as there are no nonzero elements of the form $D^2(g^{N/2})_{\bar{\alpha}\bar{\beta}\gamma\delta}$. Therefore

$$\langle q_{i\bar{j}}^{\dagger} g^{N/2} | q_{\bar{k}l}^{\dagger} g^{N/2} \rangle = 0, \quad 1 \le i < j \le s, \quad 1 \le k < l \le s . \tag{C20}$$

Type 3:

$$\langle g^{N/2} | q_{i\bar{j}} q_{kl}^{\dagger} g^{N/2} \rangle = \langle g^{N/2} | (\zeta_j a_{\bar{j}}^{\dagger} a_i + \zeta_i a_{\bar{i}}^{\dagger} a_j)(\zeta_k a_{\bar{k}}^{\dagger} a_{\bar{l}} - \zeta_l a_l^{\dagger} a_k) g^{N/2} \rangle , \tag{C21}$$

$$= \langle g^{N/2} | [-\zeta_j \bar{\zeta}_k a_{\bar{j}}^{\dagger} a_{\bar{l}}^{\dagger} a_i a_{\bar{k}} - \zeta_j \bar{\zeta}_l a_{\bar{j}}^{\dagger} (\delta_{ik} - a_{\bar{k}}^{\dagger} a_{\bar{i}}) a_{\bar{l}}$$
$$- \zeta_i \bar{\zeta}_k a_{\bar{i}}^{\dagger} a_{\bar{l}}^{\dagger} a_j a_k - \zeta_i \bar{\zeta}_l a_{\bar{i}}^{\dagger} (\delta_{jk} - a_k^{\dagger} a_j) a_l] g^{N/2} \rangle . \tag{C22}$$

Equation (C22) equals zero as no nonzero elements of the forms $D^2(g^{N/2})_{\bar{\alpha}\bar{\beta}\bar{\gamma}\delta}$, $D^2(g^{N/2})_{\alpha\beta\gamma\bar{\delta}}$, and $D^1(g^{N/2})_{\alpha\beta,\alpha\neq\beta}$ exist. Therefore

$$\langle q_{i\bar{j}}^{\dagger} g^{N/2} | q_{kl}^{\dagger} g^{N/2} \rangle = 0, \quad 1 \le i < j \le s, \quad 1 \le k < l \le s .$$

Type 4:

$$\langle g^{N/2} | q_{\bar{i}j} q_{\bar{k}l}^{\dagger} g^{N/2} \rangle = \langle g^{N/2} | (\zeta_j a_j^{\dagger} a_i + \zeta_i a_i^{\dagger} a_j)(\zeta_k a_k^{\dagger} a_{\bar{l}} + \zeta_l a_l^{\dagger} a_{\bar{k}}) g^{N/2} \rangle , \tag{C23}$$

$$= \zeta_j \bar{\zeta}_k D^2(g^{N/2})_{jk} \delta_{il} + \zeta_j \bar{\zeta}_l D^1(g_{N/2})_{jl} \delta_{ik} + \zeta_i \bar{\zeta}_k D^1(g^{N/2})_{ik} \delta_{jl}$$
$$+ \zeta_i \bar{\zeta}_l D^1(g^{N/2})_{il} \delta_{jk} - \zeta_j \bar{\zeta}_k D^2(g^{N/2})_{j\bar{l}k\bar{i}} - \zeta_j \bar{\zeta}_l D^2(g^{N/2})_{j\bar{k}l\bar{i}}$$
$$- \zeta_i \bar{\zeta}_k D^2(g^{N/2})_{i\bar{l}k\bar{j}} - \zeta_i \bar{\zeta}_l D^2(g^{N/2})_{i\bar{k}l\bar{j}} . \tag{C24}$$

By noting that $D^1(g^{N/2})_{\bar{\alpha}\bar{\alpha}} = D^1(g^{N/2})_{\alpha\alpha}$ and $D^2(g^{N/2})_{\bar{\alpha}\beta\bar{\gamma}\delta} = D^2(g^{N/2})_{\alpha\bar{\beta}\gamma\bar{\delta}}$ we see that (C24) has the same value as (C5):

$$\langle q_{\bar{i}j}^{\dagger} g^{N/2} | q_{\bar{k}l}^{\dagger} g^{N/2} \rangle = (\delta_{ik}\delta_{lj} + \delta_{il}\delta_{kj}) S_{N/2}^{-1} (\eta_i - \eta_j)^2 \sum_{1 \le i_1 < \cdots < i_{N/2-1} \le s}^{ij} \eta_{i_1} \cdots \eta_{i_{N/2-1}}$$
$$1 \le i < j \le s, \quad 1 \le k < l \le s . \tag{C25}$$

By the same algebra as the preceding, we get the final two types.

Type 5:

$$\langle q_{\bar{i}j}^{\dagger} g^{N/2} | q_{kl}^{\dagger} g^{N/2} \rangle = 0, \quad 1 \le i < j \le s, \quad 1 \le k < l \le s .$$

Type 6:

$$\langle q_{ij}^{\dagger} g^{N/2} | q_{kl}^{\dagger} g^{N/2} \rangle = \delta_{il}\delta_{jk} S_{N/2}^{-1} (\eta_i - \eta_j)^2 \sum_{1 \le i_1 < \cdots < i_{N/2-1} \le s}^{ij} \eta_{i_1} \cdots \eta_{i_{N/2-1}}, \quad 1 \le i < j \le s, \quad 1 \le k < l \le s .$$

It is interesting to note that

$$\sum_{1 \le i_1 < \cdots < i_{N/2-1} \le s}^{ij} \eta_{i_1} \cdots \eta_{i_{N/2-1}} = || \tilde{g}^{N/2-1} ||^2 , \tag{C26}$$

where

$$\tilde{g}=\sum_{1\le k\le s,k\ne i,j}\zeta_k\,|\phi_k\phi_{\bar{k}}\rangle\ . \qquad \text{(C27)}$$

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