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ORIGINAL PAPER

# Generalized P, Q and G conditions

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**Abstract** The $N$-Representability Problem entails characterizing the set of second order reduced states that are contractions of N-electron states of the Fermion Fock algebra. This problem is formulated in the form of finding the conditions that a positive linear functional defined on a subspace of this algebra must satisfy in order to be extended to the whole algebra. As this algebra is a w*-algebra one can utilize a theorem by Kadison that shows it is sufficient to consider the values of linear functionals on projectors contained in the subspace in order to determine whether they have positive extensions. Thus we find the form of projectors belonging to the subspace of one and two particle operators and subsequently show that the extension conditions needed in the $N$-Representability Problem correspond to generalized P, Q and G conditions plus the additional constraints that the functionals be dispersion free on the number operator and their values on one particle operators determined by their values on two particle operators.

**Keywords** $N$-Representability · Fock space · Positive extensions

## 1 Introduction

The $N$-Representability Problem entails finding the *necessary and sufficient conditions* that a positive trace class operator, that acts in two electron space, must satisfy in order to be the contraction of a $N$-electron state density operator and thus be a Second Order Reduced Density Operator (SORDO). It was first precisely formulated in quantum chemistry by Coleman [1] as a result of Coulsons *challenge* [2], which was inspired by work initiated by Husimi [3]. The significance of the problem derives

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from the realization that the properties of molecular systems, at a fixed geometry, are fully described by Hamiltonians that describe the kinetic energy of the individual electrons, interactions of the electrons with external and internal electric and magnetic fields and *only* the simultaneous pair wise interactions of the electrons with each other. As simultaneous three, four and higher body interactions are not significant the $N$-electron state density operator contains redundant information and the energy of molecular systems can be fully expressed in terms of the SORDO of the system, which depends on fewer variables. Hence the determination of the ground state energy can be formulated as a minimization of a linear functional over operators that act in two electron space that are *constrained* to be SORDO's, instead of a higher dimensional minimization over $N$-electron state density operators.

An intrinsic solution (i.e. only in terms of properties of operators acting in two electron space) has not been found despite a large amount of effort [4] along many complimentary pathways. This work has, however, resulted in the characterization of numerous necessary conditions (see for instance [4] and the references therein), the innovative contracted Schrödinger equation method [5] (and the references therein), [6] the relation to complexity theory [7] and various variants of the problem i.e. electron conserving/ electron nonconserving, pure/ensemble and finite/infinite dimensional.

In a paper [8] the $N$-Representability Problem was shown to be one of finding conditions for the existence of positive extensions of a linear functional from a *subspace* of an algebra to the whole algebra. Thus placing it firmly in the area of traditional mathematical analysis and allows one to utilize theorems proved in this topic over the last hundred years, where the classical Hahn–Banach theorem [9] on extensions, $\tilde{f}$, of unrestricted linear functionals, $f$, defined on subspaces, $W$, to the whole vector space $V$ was specialized to positive linear functionals defined on ordered vector spaces by Krein [10,11] and to self-adjoint subspaces of $c^*$-algebras [9] that *might or might not* contain the identity by Segal [12] and discussed in detail in [13]. In order for the extension to be a state [9] i.e. a positive normalized linear functional defined on the whole algebra its value on the identity must be one i.e.

$$\tilde{f}(I) = 1 \tag{1}$$

so if $I \in W$ then

$$\tilde{f}(I) = f(I) = 1. \tag{2}$$

Segal's theorem examines the implications of this normalization and shows that a positive normalized extension $\tilde{f}$ exists if (a)

$$f(X) \geq 0 \quad \forall X \in W_+, \tag{3}$$

where $W_+$ is the set of positive operators in $W$ i.e.

$$W_+ = \{X \in W \,|X \geq 0\}, \tag{4}$$

(b)

$$\sup_{X \in W_<} f(X) \leq 1, \tag{5}$$

where the positive part of the subspace $W$ that contains operators that are less than or equal to the identity operator is defined as

$$W_< = \{X \in W \,|\, I \geq X \geq 0\} \tag{6}$$

and (c)

$$\inf_{X \in W_>} f(X) \geq 1, \tag{7}$$

where the positive part of the subspace $W$ that contains operators that are greater than or equal to the identity operator is defined as

$$W_> = \{X \in W \,|\, X \geq I\}. \tag{8}$$

It can easily be seen that *if* $X \geq 0$ then

$$\|X\| \leq 1 \Leftrightarrow I \geq X \geq 0 \tag{9}$$

and thus

$$W_< = \{X \in W \,|\, X \in W_+;\, \|X\| \leq 1\}, \tag{10}$$

and $W_<$ is the positive part of the unit ball

$$\mathfrak{B}_1 = \{X \,|\, \|X\| \leq 1\} \tag{11}$$

contained in $W$, while $W_>$ can be expressed as

$$W_> = \{X \in W_+ \,|\, \|X\| \geq 1\} \tag{12}$$

and is the positive part of the annulus

$$\mathfrak{A}_1 = \{X \,|\, \|X\| \geq 1\} \tag{13}$$

contained in $W$.

The unit ball is a convex set and the Krein–Millmann theorem [9] shows that in a $w^*$-algebra [9] it is equal to the closure of its extreme points [14], moreover the positive part of the unit ball in a $w^*$-algebra also forms a convex set which is also the closure of *its* extreme points. In an important theorem Kadison [15], (also see the discussion in [16]), has shown that the extreme points of the positive part of the unit ball in a $w^*$-algebra are projectors and in particular belong to the unit sphere

$$\|X\| = 1. \tag{14}$$

In this paper the subspaces we need to consider do not contain any operators that belong to $W_>$ thus we only need to take into account the conditions Eqs. 3 and 5. The set $W_+$ is also a convex set and is generated by its extreme points, ext$\{W_+\}$, which is the set of projectors in $W$. A functional is positive on $W$ if and only if it is positive on ext$\{W_+\}$, while the supremum of the values of linear functionals defined on convex sets only occur at extreme points of the set, thus one has only to consider the values of the functionals on the projectors ext $\{W_+\}$ in order to ascertain whether they satisfy both conditions Eqs. 5 and 3. The *necessary and sufficient* conditions for the existence of a state that extends a linear functional defined on a subspace $W$ can thus be expressed in terms of values of the functional on the set of projectors, ext $\{W_+\}$ , as

$$1 \geq f(X) \geq 0, \quad \forall X \in \text{ext}\{W_+\}. \tag{15}$$

In the context of the $N$-Representability Problem for electrons the relevant $w^*$-algebra is the Fermion Fock algebra and the subspace is the one formed by one and two electron operators. In this paper the form of *all* the projectors in this subspace are characterized and the lower limits in Eq. 15 are shown to correspond to the well known [17] *necessary* P, Q and G conditions. The upper limits in Eq. 15 correspond to the Krein, Segal and Kadison theorems, that in conjunction with the lower limits, make the conditions *necessary and sufficient* for ensemble representability and we describe them as *generalized* P, Q and G conditions. In addition in order for a linear functional to be $N$-Representable it must also be dispersion free on the electron number operator and its values on the space of one particle operators expressed in a specific manner in terms of its values on the space of two particle operators.

In the following we discuss and examine the preceding ideas first reviewing, in Sect. 2, some mathematical concepts and notation that are utilized in the subsequent sections then in Sect. 3 the expansion and contraction maps, which are adjoints of each other, are considered in the context of Fock space [14,18], which leads to the definition of Reduced Density Operators (RDO's). In Sect. 4 we utilize the fact that the Fock algebra is a concrete realization of a $w^*$-algebra and show that RDO's correspond to Reduced States (RS's) that are positive functionals defined on self adjoint subspaces of a $w^*$-algebra that can be extended to states of the algebra. This shows that the representability problems can be formulated as finding the conditions that positive linear functionals defined on subspaces must satisfy in order to be extended to states. Kadisons theorem is then used to show that *necessary and sufficient* extension conditions can be expressed in terms of values of the functionals on projectors contained in the subspace. In Sect. 5 the form of *all* projectors that can be expressed as linear combinations of one and two electron operators is found. In Sect. 6 we display that the conditions found from Kadisons Theorem lead to generalizations of the known *necessary* P, Q and G conditions for representability and can be expressed in terms of matrix elements of first and second order reduced density matrices. In Sect. 7

we discuss the condition that must be satisfied to make the functionals and reduced density matrices ensemble $N$-representable, which leads to the list of *necessary and sufficient* ensemble $N$-representability conditions given in Sect. 8 and we conclude with a discussion in Sect. 9.

## 2 Mathematical essentials

In the following the dimension of all spaces are considered to be finite and can be thought of as approximations to the infinite dimensional case, which must be used to obtain the exact solutions of quantum mechanical equations. However notation that is appropriate for the infinite dimensional case will be used even though it becomes redundant in the finite dimensional case.

### 2.1 Fermion Fock space

We consider the Fermi Fock space, $\mathcal{H}_{\mathcal{F}}$, based on the one electron Hilbert space $\mathcal{H}^1$, defined by the direct sum

$$\mathcal{H}_{\mathcal{F}} = \bigoplus_{0 \le N \le r} \mathcal{H}^N \tag{16}$$

of the $N$-electron Hilbert spaces

$$\mathcal{H}^N = \bigwedge^{N} \mathcal{H}^1, \tag{17}$$

where $\wedge$ denotes antisymmetric tensor product and $\mathcal{H}^0 = \{\lambda\,|\phi\rangle |\, \lambda \in \mathbb{C}\}$, and $|\phi\rangle$ is the vacuum state. The inner product in the Hilbert space $\mathcal{H}_{\mathcal{F}}$ is defined as

$$\langle \Psi\,|\Phi\,\rangle_{\mathcal{F}} = \sum_{0 \le N \le r} \langle \Psi_N\,|\Phi_N\,\rangle_{\mathcal{H}^N} = \sum_{0 \le N \le r} \left\langle \Psi\,\middle|\,P_{\mathcal{H}^N}\Phi\right\rangle_{\mathcal{H}^N}, \tag{18}$$

where $P_{\mathcal{H}^N}$ is the orthogonal projector onto $\mathcal{H}^N$ and $\langle\cdot\,|\cdot\rangle_{\mathcal{H}^N}$ is the inner product in this Hilbert space. (Notational note: If the domain of $\langle\cdot\,|\cdot\rangle_{\mathcal{H}^N}$ is obvious from the context the subscript "$\mathcal{H}^N$" will not be explicitly shown).

### 2.2 Fermion fock algebra

The fermion Fock algebra, $\mathcal{F}$, is the space of bounded operators ("Appendix A") acting in $\mathcal{H}_{\mathcal{F}}$ i.e.

$$\mathcal{F} = \mathcal{B}\left(\mathcal{H}_{\mathcal{F}}\right). \tag{19}$$

This space can be generated by polynomials

$$X = \sum_{0 \le P, Q \le r} \sum_{\substack{1 \le j_1 < \cdots < j_P \le r \\ 1 \le k_1 < \cdots < k_Q \le r}} X_{j_1 \ldots j_P k_1 \ldots k_P} a_{j_1}^{\dagger} \ldots a_{j_P}^{\dagger} a_{k_Q} \ldots a_{k_1} \tag{20}$$

of second quantized operators, $\left\{ a_j^{\dagger} \middle| 1 \le j \le r \right\}$, which are defined by their action on the vacuum vector $|\phi\rangle$ by

$$a_j^{\dagger} |\phi\rangle = \left|\varphi_j\right\rangle, \quad 1 \le j \le r, \tag{21}$$

where $\left\{ \left|\varphi_j\right\rangle \middle| 1 \le j \le r \right\}$ is a complete orthonormal basis of the one-electron space $\mathcal{H}^1$ and satisfy the anti-commutation relationships given by

$$\left[a_j^{\dagger}, a_k\right]_+ = a_j^{\dagger} a_k + a_k a_j^{\dagger} = \delta_{jk}; \quad 1 \le j, k \le r. \tag{22}$$

The fermion Fock algebra can be decomposed as a vector space direct sum

$$\mathcal{F} = \mathcal{F}_e \oplus \mathcal{F}_0 \tag{23}$$

of a electron conserving subalgebra $\mathcal{F}_e$ and a electron non conserving subspace of operators $\mathcal{F}_0$. The subalgebra $\mathcal{F}_e$ can be further decomposed as a direct sum of subspaces

$$\mathcal{F}_e = \bigoplus_{0 \le N \le r} \mathcal{B}\left(\mathcal{H}_{\mathcal{F}}\right)_N, \tag{24}$$

where

$$\mathcal{B}\left(\mathcal{H}_{\mathcal{F}}\right)_N = \left\{ \sum_{\substack{1 \le j_1 < \cdots < j_N \le r \\ 1 \le k_1 < \cdots < k_N \le r}} X_{j_1 \ldots j_N k_1 \ldots k_N} a_{j_1}^{\dagger} \ldots a_{j_N}^{\dagger} a_{k_N} \ldots a_{k_1} \right\} \tag{25}$$

or as a direct sum of subalgebras

$$\mathcal{F}_e = \bigoplus_{0 \le N \le r} \mathcal{B}\left(\mathcal{H}^N\right), \tag{26}$$

where $\mathcal{B}\left(\mathcal{H}^N\right)$ is the space of bounded operators acting in $\mathcal{H}^N$. The subspace $\mathcal{F}_0$ can be decomposed as the vector space direct sum

$$\mathcal{F}_o = \bigoplus_{0 \le N \ne M \le r} \mathcal{B}\left(\mathcal{H}_{\mathcal{F}}\right)_{N,M}, \tag{27}$$

where

$$\mathcal{B}\left(\mathcal{H}_{\mathcal{F}}\right)_{N,M} = \left\{ \sum_{\substack{1\leq j_1<\cdots<j_N\leq r \\ 1\leq k_1<\cdots<k_M\leq r}} X_{j_1\ldots j_N k_1\ldots k_M} a_{j_1}^{\dagger}\ldots a_{j_N}^{\dagger} a_{k_M}\ldots a_{k_1} \right\} \tag{28}$$

or as the vector space direct sum

$$\mathcal{F}_o = \bigoplus_{0\leq N\neq M\leq r} \mathcal{B}\left(\mathcal{H}^N, \mathcal{H}^M\right), \tag{29}$$

where $\mathcal{B}\left(\mathcal{H}^N, \mathcal{H}^M\right)$ is the vector space of bounded linear maps from the Hilbert space $\mathcal{H}^N$ to the Hilbert space $\mathcal{H}^M$. The decompositions Eqs. 24 and 27 express the fermion Fock algebra in *second quantized* form as polynomials of second quantized operators, while the decompositions Eqs. 26 and 29 express it in *first quantized* form as expansions of the ket-bras

$$\left\{ \left|\varphi_{j_1}\ldots\varphi_{j_N}\right\rangle\left\langle\varphi_{k_1}\ldots\varphi_{k_M}\right| \middle| 1\leq j_1<\cdots<j_N\leq r, 1\leq k_1<\cdots<k_M\leq r; \right.$$
$$\left. 0\leq N, M\leq r\right\} \tag{30}$$

## 2.3 Operator inner product

The Fock space trace operation is defined as

$$\mathrm{Tr}\left\{X\right\} = \sum_{0\leq N\leq r}\ \sum_{1\leq j_1<\cdots<j_N\leq r} \left\langle \Psi_{N j_1\ldots j_N} \middle| X\Psi_{N j_1\ldots j_N}\right\rangle, \tag{31}$$

where $\left\{\Psi_{N j_1\ldots j_N} \middle| 1\leq j_1<\cdots<j_N\leq r; 0\leq N\leq r\right\}$ are complete orthonormal bases for $\mathcal{H}^N, 0\leq N\leq r$. One can use this trace operation to define the space of trace class operators $\mathcal{B}_1\left(\mathcal{H}_{\mathcal{F}}\right)$ that have finite trace for all bases and the space of Hilbert Schmidt operators $\mathcal{B}_2\left(\mathcal{H}_{\mathcal{F}}\right)$ that form a Hilbert space with inner product

$$\left(X\left|Y\right.\right) = \mathrm{Tr}\left\{X^{\dagger}Y\right\}. \tag{32}$$

In finite dimensions, i.e. $r<\infty$, there is no distinction between these spaces of operators i.e. $\mathcal{B}\left(\mathcal{H}_{\mathcal{F}}\right) = \mathcal{B}_1\left(\mathcal{H}_{\mathcal{F}}\right) = \mathcal{B}_2\left(\mathcal{H}_{\mathcal{F}}\right)$.

# 3 Expansion and contraction maps

The expansion and contraction maps relate the first and second quantization formulation of quantum mechanics and are defined by the following:

### 3.1 Contraction map

Employing the work of [18] one can define a *non singular* generalized contraction map

$$L : \mathcal{B}_1(\mathcal{H}_\mathcal{F}) \to \mathcal{B}_1(\mathcal{H}_\mathcal{F}) \tag{33}$$

by

$$L(Y) = \sum_{0\le N,M\le r} \sum_{\substack{1\le j_1<\cdots<j_M\le r\\ 1\le k_1<\cdots<k_N\le r}} \left(a^\dagger_{k_1}\ldots a^\dagger_{k_N} a_{j_M}\ldots a_{j_1}\middle| Y\right) \left|\varphi_{j_1}\ldots\varphi_{j_M}\right\rangle\left\langle\varphi_{k_1}\ldots\varphi_{k_N}\right|. \tag{34}$$

### 3.2 Expansion map

The expansion map

$$\Gamma : \mathcal{B}(\mathcal{H}_\mathcal{F}) \to \mathcal{B}(\mathcal{H}_\mathcal{F}) \tag{35}$$

is adjoint to the contraction map, i.e. $\Gamma = L^\dagger$, with respect to inner product $(\cdot\,|\cdot)$ and is defined by

$$(\Gamma(X)\,|Y) = (X\,|L(Y)) \quad \forall Y \in \mathcal{B}_1(\mathcal{H}_\mathcal{F}). \tag{36}$$

One can show ("Appendix B.2.1") that $\Gamma$ is *actually the second quantization map*

$$a^\dagger_{j_1}\ldots a^\dagger_{j_N} a_{k_P}\ldots a_{k_M} = \Gamma\left(\left|\varphi_{j_1}\ldots\varphi_{j_M}\right\rangle\left\langle\varphi_{k_1}\ldots\varphi_{k_N}\right|\right), \tag{37}$$

which can be expressed in terms of exterior multiplication by the identity operator in $\mathcal{F}$ as

$$\Gamma\left(\left|\varphi_{j_1}\ldots\varphi_{j_M}\right\rangle\left\langle\varphi_{k_1}\ldots\varphi_{k_N}\right|\right) = \left|\varphi_{j_1}\ldots\varphi_{j_M}\right\rangle\left\langle\varphi_{k_1}\ldots\varphi_{k_N}\right| \wedge I_{\mathcal{H}_\mathcal{F}}. \tag{38}$$

The expansion and contraction maps transform naturally between the first and second quantization direct sum decompositions of $\mathcal{F}$ i.e.

$$\Gamma : \bigoplus_{0\le N,M\le r} \mathcal{B}\left(\mathcal{H}^N, \mathcal{H}^M\right) \to \bigoplus_{0\le N,M\le r} \mathcal{B}(\mathcal{H}_\mathcal{F})_{N,M} \tag{39}$$

and

$$L : \bigoplus_{0\le N,M\le r} \mathcal{B}(\mathcal{H}_\mathcal{F})_{N,M} \to \bigoplus_{0\le N,M\le r} \mathcal{B}\left(\mathcal{H}^N, \mathcal{H}^M\right). \tag{40}$$

### 3.3 Reduced density operators

The $P$th order reduced density operator associated with a state $D \in S_{\mathcal{F}}$ can be defined by using the contraction map $L$ as

$$D_P = P_{\mathcal{H}^P} L(D) P_{\mathcal{H}^P} = \sum_{\substack{1 \le j_1 < \cdots < j_P \le r \\ 1 \le k_1 < \cdots < k_P \le r}} \left( a_{k_1}^{\dagger} \ldots a_{k_P}^{\dagger} a_{j_1} \ldots a_{j_P} \middle| D \right) \left| \varphi_{j_1} \ldots \varphi_{j_P} \right\rangle \left\langle \varphi_{k_1} \ldots \varphi_{k_P} \right| \tag{41}$$

and in particular the SORDO is given by

$$D_2 = P_{\mathcal{H}^2} L(D) P_{\mathcal{H}^2} = \sum_{\substack{1 \le j_1 < j_2 \le r \\ 1 \le k_1 < k_2 \le r}} \left( a_{k_1}^{\dagger} a_{k_2}^{\dagger} a_{j_1} a_{j_2} \middle| D \right) \left| \varphi_{j_1} \varphi_{j_2} \right\rangle \left\langle \varphi_{k_1} \varphi_{k_2} \right|. \tag{42}$$

If $D$ is a state describing a system of $N$ electrons then

$$\begin{aligned} D &= D^N = P_{\mathcal{H}^N} D P_{\mathcal{H}^N} \\ P_{\mathcal{H}^M} D P_{\mathcal{H}^M} &= 0,\ M \neq N \end{aligned} \tag{43}$$

and the above construction corresponds to the normalization

$$\mathrm{Tr}\{D_2\} = \binom{N}{2}. \tag{44}$$

## 4 Extensions of positive functionals

The Fermion Fock algebra is a concrete realization of a $w^*$-algebra [9] (that contains an identity element), which is a $c^*$-algebra that also has the property of being a dual space of another Banach space, in this case $\mathcal{B}(\mathcal{H}_{\mathcal{F}})$ is the dual space of $\mathcal{B}_1(\mathcal{H}_{\mathcal{F}})$ i.e. $\mathcal{B}_1(\mathcal{H}_{\mathcal{F}})^*$. The important property of $w^*$-algebras vis-à-vis $c^*$-algebras is that they are the closure of their idempotents, which in the case of $\mathcal{F}$ are the orthogonal projectors onto subspaces of $\mathcal{H}_{\mathcal{F}}$.

### 4.1 States

A state on a $w^*$-algebra is a bounded positive linear function, $f$, such that $f(I) = 1$, where $I$ is the identity element of the algebra, it is called a normal state if it can be identified with an element of the predual of the algebra otherwise it is an abnormal state. In this paper only normal states belonging to the predual $\mathcal{B}_1(\mathcal{H}_{\mathcal{F}})$ of $\mathcal{B}(\mathcal{H}_{\mathcal{F}})$ are considered. In the Fermion Fock algebra normal states are in one to one correspondence with normalized density operators i.e.

$$f(X) = \mathrm{Tr}\left\{X D_f\right\}; \quad D_f \in S_{\mathcal{F}}. \tag{45}$$

The convex set, $S_{\mathcal{F}}$, of density operators in $\mathcal{F}$ is given by

$$S_{\mathcal{F}} = \{D \,|D \in \mathcal{B}_1 (\mathcal{H}_{\mathcal{F}})\,;\, D \geq 0; \mathrm{Tr}\, D = 1\}\,, \tag{46}$$

whose elements could describe any type of physical state i.e. electron conserving or non conserving, ensemble or pure etc.

### 4.2 Partial states

A *partial* state is a positive linear functional defined on a self adjoint subspace, $\mathcal{W}$, of a $w^*$-algebra *that contains* the identity $I$ and is a restriction of a state. It can be shown [19,10] that the necessary and sufficient condition for a positive linear functional defined on such a subspace $\mathcal{W}$ to be a partial state and thus extended to a state is

$$\sup_{\substack{I \geq X \geq 0 \\ X \in \mathcal{W}}} f(X) \leq 1 \tag{47}$$

and

$$\inf_{\substack{X \geq I \\ X \in \mathcal{W}}} f(X) \geq 1. \tag{48}$$

The identity element $I_{\mathcal{H}_{\mathcal{F}}}$ of $\mathcal{B}(\mathcal{H}_{\mathcal{F}})$ can be expanded as

$$I_{\mathcal{H}_{\mathcal{F}}} = \sum_{0 \leq N \leq r} P_{\mathcal{H}^N}\,, \tag{49}$$

where $P_{\mathcal{H}^N}$ are the orthogonal projectors onto $\mathcal{H}^N$, $0 \leq N \leq r$ and in particular $P_{\mathcal{H}^0} = |\phi\rangle\langle\phi|$ is the projector onto the vacuum state. Thus the condition Eq. 48 only effects operators that are non zero on the vacuum state.

### 4.3 Reduced states

A *reduced* state is a postive linear functional defined on a self adjoint subspace of a $w^*$-algebra *that does not contain* the identity and is a restriction of a state. The necessary and sufficient condition [12] for a linear functional defined on such a subspace $\mathcal{W}$ to be a reduced state and thus be extended to a state is

$$1 \geq f(X) \geq 0, \quad \forall X \in \mathfrak{B}_{1+}(\mathcal{W})\,, \tag{50}$$

where $\mathfrak{B}_{1+}(\mathcal{W})$ is the positive part of the unit ball of $\mathcal{B}(\mathcal{H}_{\mathcal{F}})$ contained in $W$ given by

$$\mathfrak{B}_{1+}(\mathcal{W}) = \{X|\, X \in \mathcal{W}, I \geq X \geq 0\} \equiv \left\{X|\, X \in \mathcal{W}_+, \|X\|_{\mathcal{B}(\mathcal{H}_{\mathcal{F}})} \geq 1\right\} \tag{51}$$

and

$$\inf_{X\in\mathfrak{A}_{1+}(\mathcal{W})} f(X) \geq 1, \tag{52}$$

where $\mathfrak{A}_{1+}(\mathcal{W})$ is the positive part of the unit annulus of $\mathcal{B}(\mathcal{H}_{\mathcal{F}})$ contained in $W$ given by

$$\mathfrak{A}_{1+}(\mathcal{W}) = \{X|\, X \in \mathcal{W}, X \geq I\} \equiv \left\{X|\, X \in \mathcal{W}_{+}, \|X\|_{\mathcal{B}(\mathcal{H}_{\mathcal{F}})} \leq 1\right\}. \tag{53}$$

An extension of an important theorem of Kadison [15] applied to self adjoint subspaces of $w^{*}$-algebra shows that the positive extension condition Eq. 51 can be expressed in terms of projectors belonging $\mathcal{W}$, an observation that is crucial in deriving necessary and sufficient conditions for representability (Sect. 5).

In order to obtain representability conditions for SORDO's the appropriate subspace to consider in $\mathcal{B}(\mathcal{H}_{\mathcal{F}})$ is the subspace formed by one and two electron conserving operators

$$\Lambda_2 = \bigoplus_{1\leq P\leq 2} \mathcal{B}(\mathcal{H}_{\mathcal{F}})_P\,, \tag{54}$$

as reduced states defined on $\Lambda_2$ correspond to SORDO's through

$$D_2 = \sum_{\substack{1\leq j_1<j_2\leq r\\ 1\leq k_1<k_2\leq r}} f\left(a^{\dagger}_{j_1}a^{\dagger}_{j_2}a_{k_2}a_{k_1}\right)\left|\varphi_{j_1}\varphi_{j_2}\right\rangle\left\langle\varphi_{k_1}\varphi_{k_2}\right|, \tag{55}$$

where

$$f\left(a^{\dagger}_{j_1}a^{\dagger}_{j_2}a_{k_2}a_{k_1}\right) = \left(a^{\dagger}_{k_1}a^{\dagger}_{k_2}a_{j_2}a_{j_1}\middle|\, D\right) \tag{56}$$

and FORDO's through

$$D_1 = \sum_{\substack{1\leq j_1\leq r\\ 1\leq k_1\leq r}} f\left(a^{\dagger}_{j_1}a_{k_1}\right)\left|\varphi_{j_1}\right\rangle\left\langle\varphi_{k_1}\right|, \tag{57}$$

where

$$f\left(a^{\dagger}_{j_1}a_{k_1}\right) = \left(a^{\dagger}_{k_1}a_{j_1}\middle|\, D\right). \tag{58}$$

In $\mathcal{B}(\mathcal{H}_{\mathcal{F}})$ the condition Eq. 53 only effects operators that are non zero on the vacuum state thus does not constrain any operators belonging to $\Lambda_2$ and one can just concentrate on the conditions given by Eq. 51.

## 5 Projectors

As we are searching for necessary and sufficient conditions for extending positive *linear* functionals the condition Eq. 5 needs only to be checked on extreme points of the positive portion of the unit ball $\mathfrak{B}_1(\Lambda_2)$ , which are projection operators [15]. One should note that these conditions will be representability conditions and that further constraints need to considered (Sect. 8) to obtain $N$-representability conditions. Projectors in $\mathcal{B}(\mathcal{H}_{\mathcal{F}})$ are postive idempotent operators, $P$, with norm equal to one i.e.

$$\begin{aligned} P &\geq 0 \\ P^2 &= P \\ \|P\|_{\mathcal{B}(\mathcal{H}_F)} &= \sup_{|\Psi\rangle\in\mathcal{H}_{\mathcal{F}}} \left\{ \frac{\langle\Psi\,|P\Psi\rangle}{\langle\Psi\,|\Psi\rangle} \right\} = 1. \end{aligned} \tag{59}$$

We first characterize the projectors in $\mathcal{B}(\mathcal{H}_{\mathcal{F}})_1$ , then $\mathcal{B}(\mathcal{H}_{\mathcal{F}})_2$ and finally $\Lambda_2$.

Projectors in $\mathcal{B}(\mathcal{H}_{\mathcal{F}})_1$

Every positive operator in $\mathcal{B}(\mathcal{H}_{\mathcal{F}})_1$ can be expressed as (“Appendix B”)

$$\lambda_1 = \sum_{1\leq j,k\leq r} \lambda_{1jk} a_j^{\dagger} a_k = \sum_{1\leq l\leq r} \beta_l b_l^{\dagger} b_l,\ \beta_l \geq 0, 1 \leq l \leq r, \tag{60}$$

where

$$b_l^{\dagger} = \sum_{1\leq j\leq r} u_{lj} a_j^{\dagger}, \quad 1 \leq l \leq r \tag{61}$$

and the coefficients $\{u_{lj}\}$ form a $r \times r$ unitary matrix i.e.

$$\mathbb{U}^{\dagger}\mathbb{U} = \mathbb{U}\mathbb{U}^{\dagger} = \mathbb{I}_r. \tag{62}$$

In “Appendix A” we show that the idempotency condition

$$\left(\sum_{1\leq l\leq r} \beta_l b_l^{\dagger} b_l\right)^2 = \sum_{1\leq l\leq r} \beta_l b_l^{\dagger} b_l \tag{63}$$

together with the norm condition

$$\left\| \sum_{1\leq l\leq r} \beta_l b_l^{\dagger} b_l \right\|_{\mathcal{B}(\mathcal{H}_{\mathcal{F}})} = 1 \tag{64}$$

can only be satisfied by positive operators where

$$\beta_l = 0,\ 1 \le l \ne k \le r \tag{65}$$

for some fixed $k$. Thus all projectors belonging to $\mathcal{B}\,(\mathcal{H}_{\mathcal{F}})_1$ are of the form

$$\lambda_1 = b^\dagger b, \tag{66}$$

where $b^\dagger$ creates a normalized General Spin Orbital (GSO)

Projectors in $\mathcal{B}(\mathcal{H}_{\mathcal{F}})_2$

Every positive operator in $\mathcal{B}\,(\mathcal{H}_{\mathcal{F}})_2$ can be expressed as ("Appendix B")

$$\lambda_2 = \sum_{\substack{1\le j<k\le r\\ 1\le l<m\le r}} \lambda_{2\,jklm} a_j^\dagger a_k^\dagger a_m a_l = \sum_{1\le l\le\binom{r}{2}} \beta_l g_l^\dagger g_l,\ \beta_l \ge 0, 1 \le l \le \binom{r}{2}, \tag{67}$$

where the geminal creator is

$$g_l^\dagger = \sum_{1\le j<k\le r} u_{ljk} a_j^\dagger a_k^\dagger, \quad 1 \le l \le \binom{r}{2} \tag{68}$$

and the coefficients $\left\{u_{ljk}\middle|\, 1 \le l \le \binom{r}{2}, 1 \le j < k \le r\right\}$ form a $\binom{r}{2} \times \binom{r}{2}$ unitary matrix i.e.

$$\mathbb{U}^\dagger\mathbb{U} = \mathbb{U}\mathbb{U}^\dagger = \mathbb{I}_{\binom{r}{2}}. \tag{69}$$

In "Appendix B" we show that the idempotency condition

$$\left(\sum_{1\le l\le\binom{r}{2}} \beta_l g_l^\dagger g_l\right)^2 = \sum_{1\le l\le\binom{r}{2}} \beta_l g_l^\dagger g_l \tag{70}$$

together with the norm condition

$$\left\|\sum_{1\le l\le\binom{r}{2}} \beta_l g_l^\dagger g_l\right\|_{\mathcal{B}(\mathcal{H}_{\mathcal{F}})} = 1 \tag{71}$$

can only be satisfied by positive operators where

$$\beta_l = 0,\ 1 \le l \ne k \le \binom{r}{2} \tag{72}$$

for some fixed $k$ and the rank of the $k$th geminal must be one. Thus in order that a two electron operator $\lambda_2$ be a projection operator it must be of the form

$$\lambda_2 = a^\dagger b^\dagger ba, \tag{73}$$

where $a^\dagger$ and $b^\dagger$ create normalized orthogonal GSO's.

Projectors in $\Lambda_2$

### 5.1 Projections from two hole operators

By considering the positivity, idempotency and normalization relationship for two *hole* operators

$$\eta_2 = \sum_{\substack{1\le j<k\le r\\ 1\le l<m\le r}} \eta_{2jklm} a_j a_k a_m^\dagger a_l^\dagger = \sum_{1\le l\le \binom{r}{2}} \gamma_l h_l h_l^\dagger,\ \gamma_l \ge 0,\ 1\le l\le \binom{r}{2}, \tag{74}$$

where the geminal annihilator is

$$g_l = \sum_{1\le j<k\le r} u_{2ljk} a_j a_k,\ 1\le l\le \binom{r}{2} \tag{75}$$

and the coefficients $\left\{u_{2ljk} \middle| 1\le l\le \binom{r}{2}, 1\le j<k\le r\right\}$ form a $\binom{r}{2}\times\binom{r}{2}$ unitary matrix i.e.

$$\mathbb{U}_2^\dagger \mathbb{U}_2 = \mathbb{U}_2 \mathbb{U}_2^\dagger = \mathbb{I}_{\binom{r}{2}}, \tag{76}$$

one can carry out the same analysis as in Sect. 5 and obtain ("Appendix B") that in order that the two hole operator $\eta_2$ be a projection operator it must be of the form

$$\eta_2 = baa^\dagger b^\dagger, \tag{77}$$

where $a$ and $b$ annihilate normalized orthogonal GSO's. The projection operator $\eta_2$ does not belong to $\mathcal{B}(\mathcal{H}_\mathcal{F})_2$ but by using the canonical anticommutation relationships Eq. 22 one can observe that

$$\eta_2 = baa^\dagger b^\dagger = I_{\mathcal{H}_\mathcal{F}} - a^\dagger a - b^\dagger b + a^\dagger b^\dagger ba \tag{78}$$

and thus

$$a^\dagger a + b^\dagger b - a^\dagger b^\dagger ba = I_{\mathcal{H}_\mathcal{F}} - \eta_2, \tag{79}$$

which shows that

$$\tilde{\lambda}_2 = a^\dagger a + b^\dagger b - a^\dagger b^\dagger ba \tag{80}$$

is a projection operator that belongs to $\Lambda_2$.

### 5.2 Projections from products of one electron operators

By considering the positivity, idempotency and normalization relationships for products $\lambda_1\lambda_1'$ of one electron operators of the form Eq. 60 one can determine ("Appendix B") that these products are projection operators when

$$\lambda_1\lambda_1' = a^\dagger bb^\dagger a = a^\dagger a - a^\dagger b^\dagger ba. \tag{81}$$

One can prove ("Appendix B") that there are no other projection operators of the form

$$\lambda = \sum_{1\le j,k\le r} \lambda_{1jk} a_j^\dagger a_k + \sum_{\substack{1\le j<k\le r\\ 1\le l<m\le r}} \lambda_{2jklm} a_j^\dagger a_k^\dagger a_m a_l \tag{82}$$

other than

$$a^\dagger a,\ a^\dagger b^\dagger ba,\ a^\dagger a - a^\dagger b^\dagger ba,\ a^\dagger a + b^\dagger b - a^\dagger b^\dagger ba. \tag{83}$$

## 6 Generalized P, Q and G conditions

The necessary P, Q and G conditions for representability of a $\binom{r}{2} \times \binom{r}{2}$ hermitian matrices were quickly discovered [17]. These conditions can be expressed in terms of the basic variables of the ground state energy optimization problem formed by the complex matrix elements $\left\{ D_{2j_1j_2k_1k_2} \middle| 1 \le j_1 < j_2 \le r, 1 \le k_1 < k_2 \le r \right\}$ of the matrix $\mathbb{D}_2$. In the notation of this paper they are:

### 6.1 P-Condition

A potential Second Order Reduced Density Matrix (SORDM) matrix $\mathbb{D}_2$ given by

$$D_{2j_1j_2k_1k_2} = \left( a_{k_1}^\dagger a_{k_2}^\dagger a_{j_1} a_{j_2} \middle| D \right) = \overline{D_{2k_1k_2j_1j_2}} \tag{84}$$

is semi definite i.e.

$$\mathbb{D}_2 \ge 0. \tag{85}$$

6.2 Q-Condition

The matrix $\mathbb{Q}$ given by

$$Q_{j_1 j_2 k_1 k_2} = \left(a^{\dagger}_{k_1} a_{j_1} a^{\dagger}_{k_2} a_{j_2} \middle| D\right) = \overline{Q_{k_1 k_2 j_1 j_2}} \tag{86}$$

is semi definite i.e.

$$\mathbb{Q} \geq 0. \tag{87}$$

If one invokes the pure $N$ condition (Sect. 8) this condition becomes a necessary $N$-representability condition and the $\mathbb{Q}$ matrix can be expressed in terms of the matrix $\mathbb{D}_2$ as

$$Q_{j_1 j_2 k_1 k_2} = \frac{1}{(N-1)} \sum_{1 \leq l \leq r} D_{2 j_2 l k_1 l} \delta_{j_1 k_2} - D_{2 j_1 j_2 k_1 k_2}. \tag{88}$$

6.3 G-Condition

The matrix $\mathbb{G}_2$ given by

$$G_{j_1 j_2 k_1 k_2} = \left(a_{j_1} a_{j_2} a^{\dagger}_{k_1} a^{\dagger}_{k_2} \middle| D\right) = \overline{G_{2 k_1 k_2 j_1 j_2}} \tag{89}$$

is semi definite i.e.

$$\mathbb{G} \geq 0. \tag{90}$$

Again if one invokes the pure $N$ condition (Sect. 8) this condition becomes a necessary $N$-representability condition and the $\mathbb{G}$ matrix can be expressed in terms of the matrix $\mathbb{D}_2$ as

$$G_{j_1 j_2 k_1 k_2} = \frac{1}{(N-1)} \sum_{1 \leq l \leq r} \left\{ D_{2 j_2 l k_1 l} \delta_{j_1 k_2} + D_{2 j_1 l k_2 l} \delta_{j_2 k_1} \right\} - D_{2 j_1 j_2 k_1 k_2}. \tag{91}$$

The following generalized P, Q and G conditions, produced by examining the values of the functional $f$ on projectors belonging to $\Lambda_2$, in combination with the one electron conditions

$$1 \geq f\left(b^{\dagger} b\right) \geq 0 \, \forall b, \tag{92}$$

are *Necessary and Sufficient* for the existence of positive extensions of bounded linear functionals

$$f : \Lambda_2 \rightarrow \mathbb{C} \tag{93}$$

to a state of $\mathcal{B}(\mathcal{H}_{\mathcal{F}})$ and are based on the theorems of Krien [10], Segal [12] and Kadison [15].

### 6.4 Generalized P-Condition

A linear functional $f$ can be extended to a state if

$$1 \geq f\left(a^{\dagger}b^{\dagger}ba\right) \geq 0\,\forall a, b, \tag{94}$$

where $|a\rangle$ and $|b\rangle$ are normalized orthogonal GSO's belonging to $\mathcal{H}^1$ and $a^{\dagger}$ and $b^{\dagger}$ are the creators of those GSO's. As

$$D_{2abab} = f\left(a^{\dagger}b^{\dagger}ba\right) \tag{95}$$

this is a *necessary* condition for ensemble representability.

### 6.5 Generalized Q-Condition

A linear functional $f$ can be extended to a state if

$$1 \geq f\left(a^{\dagger}a - a^{\dagger}b^{\dagger}ba\right) \geq 0\,\forall a, b, \tag{96}$$

which gives

$$1 \geq D_{1aa} - D_{2abab} \geq 0\,\forall a, b, \tag{97}$$

where the diagonal elements of a possible First Order Reduced Density Matrix (FORDM) are defined as

$$D_{1aa} = f\left(a^{\dagger}a\right). \tag{98}$$

Again this is a *necessary* condition for ensemble representability.

### 6.6 Generalized G-Condition

A linear functional $f$ can be extended to a state if

$$1 \geq f\left(a^{\dagger}a + b^{\dagger}b - a^{\dagger}b^{\dagger}ba\right) \geq 0\,\forall a, b, \tag{99}$$

which gives

$$1 \geq D_{1aa} - D_{1bb} - D_{2abab} \geq 0\, \forall a, b \tag{100}$$

and also a *necessary* condition for ensemble representability.

## 7 Electron and pair number conditions

In order to obtain $N$-representable extensions one must constrain the functional $f$ to be dispersion free on the number operator i.e.

$$f\left(\mathcal{N}_1^2\right) = f\left(\mathcal{N}_1\right)^2, \tag{101}$$

where

$$\mathcal{N}_1 = \sum_{1 \leq j \leq r} a_j^{\dagger} a_j. \tag{102}$$

One can show ("Appendix B.2.1") that Eq. 101 is equivalent to

$$f\left(\mathcal{N}_1\right) = N \tag{103}$$

and

$$f\left(\mathcal{N}_2\right) = \binom{N}{2} \tag{104}$$

for some fixed $N$, where the pair operator $\mathcal{N}_2$ is defined as

$$\mathcal{N}_2 = \sum_{1 \leq j < k \leq r} a_j^{\dagger} a_k^{\dagger} a_k a_j. \tag{105}$$

If $f$ is dispersion free on the number operator the values of $f$ on $\mathcal{B}\left(\mathcal{H}_{\mathcal{F}}\right)_1$ must be related to its values on $\mathcal{B}\left(\mathcal{H}_{\mathcal{F}}\right)_2$ by

$$f\left(a_j^{\dagger} a_k\right) = (N-1)^{-1} f\left(a_j^{\dagger} \mathcal{N}_1 a_k\right) = (N-1)^{-1} \sum_{1 \leq l \leq r} f\left(a_j^{\dagger} a_l^{\dagger} a_l a_k\right), \tag{106}$$

thus if the functional is only defined on $\mathcal{B}\left(\mathcal{H}_{\mathcal{F}}\right)_2$ one can define allowable extensions to $\mathcal{B}\left(\mathcal{H}_{\mathcal{F}}\right)_1$ by Eq. 106.

In terms of matrix elements the definition Eq. 106 becomes

$$D_{1jk} = (N-1)^{-1} \sum_{1 \leq l \leq r} D_{2jlkl} \tag{107}$$

and one can see that if the value of the functional on the pair operator is set by Eq. 104 then the electron number condition Eq. 103 is automatically ensured.

## 8 *N*-Representability conditions

The representability conditions in Sect. 6 can be complimented and modified by the conditions in Sect. 7 to form ensemble *Necessary and Sufficient* $N$-representability conditions which are:

1. Normalization

$$\sum_{1\leq j<k\leq r} D_{2jkjk} = \binom{N}{2} \tag{108}$$

2. Generalized P-Condition

$$1 \geq D_{2abab} \geq 0\, \forall a, b \tag{109}$$

3. Generalized Q-Condition

$$1 \geq (N-1)^{-1} \sum_{1\leq l\leq r} D_{2alal} - D_{2abab} \geq 0\, \forall a, b \tag{110}$$

4. Generalized G-Condition

$$1 \geq (N-1)^{-1} \sum_{1\leq l\leq r} \{D_{2alal} + D_{2blbl}\} - D_{2abab} \geq 0\, \forall a, b. \tag{111}$$

The conditions Eqs. 108,109,111 and the lower bound in Eq. 110 have been discovered in the study of the Diagonal Representability Problem [20–24]. However, these conditions were not caste in terms of bounds on the extremal values of a linear functional on the intersection of the unit ball of the Fermion Fock algebra with the subspace $\Lambda_2$. Expressing the bounds in this context allows one to utilize general extension theorems from functional analysis to determine necessary and sufficient conditions for a linear functional to be a reduced state *if all the projectors in this intersection are characterized*. The theorems in "Appendix B" characterize all these projections.

## 9 Discussion

In this paper we have described how the $N$-Representability problem entails finding the conditions that linear functionals belonging to the dual space, $\mathcal{B}(\mathcal{H}_{\mathcal{F}})_2^*$, of bounded linear functionals defined on the subspace of second quantized two electron operators, $\mathcal{B}(\mathcal{H}_{\mathcal{F}})_2$, contained in the Fock algebra, $\mathcal{F}$, need to satisfy in order to be extended to $N$-electron states and thus be reduced $N$-electron states i.e. restrictions of $N$-electron states.

As this algebra is a $w^*$-algebra the theorems of Krein, Segal and Kadison were utilized to show that the positive extension conditions could be expressed in terms of the values of the restricted linear functionals on projectors contained in the subspace $\Lambda_2$ generated by the one and two electron operators, i.e. on the extreme points, ext $\{\Lambda_{2+}\}$, of the cone of positive operators belonging to this space, which have to belong to the interval $[0, 1]$. These conditions are generalizations of the known P, Q and G conditions, which are given by the lower bound of this interval. In addition the condition that these functionals be restrictions of $N$-electron states entails that they must be dispersion free on the number operator, $\mathcal{N}_1$, and that their values on the one electron subspace $\mathcal{B}(\mathcal{H}_{\mathcal{F}})_1$ be determined by their values on the two electron subspace $\mathcal{B}(\mathcal{H}_{\mathcal{F}})_2$.

We also described how the functionals belonging to $\mathcal{B}(\mathcal{H}_{\mathcal{F}})_2^*$ correspond to operators belonging $\mathcal{B}\left(\mathcal{H}^2\right)$ that act in $\mathcal{H}^2$ and obtained their matrix representations in a natural way using the generalized contraction map. This map is the adjoint of the generalized expansion map which we display is the second quantization map. This correspondence shows that the $N$-electron ground state of the system can be determined by a constrained variation of the linear functional that corresponds to the reduced Hamiltonian, over operators belonging to $\mathcal{B}\left(\mathcal{H}^2\right)$ subject to the normalization and generalized P, Q and G constraints, which are all linear. This problem can be expressed in terms of matrix elements of operators belonging $\mathcal{B}\left(\mathcal{H}^2\right)$ produced by decomposable bases of $\mathcal{H}^2$, however in order to be sufficient conditions the matrix elements must satisfy them in *all decomposable* bases, i.e. the conditions on the matrices produced by these elements must be conserved under the under the action of the representations, $\mathcal{R}_{\mathcal{H}^2}\left(U\left(\mathcal{H}^1\right)\right)$, of the one electron unitary group $U\left(\mathcal{H}^1\right)$ on $\mathcal{H}^2$. These observations can also be used to obtain to a more constrained form of the Semi Definite Programming (SDP) method successfully used by Mazziotti [25].

In a future work this variational problem will be expressed in terms of functions defined on the group manifold of $U\left(\mathcal{H}^1\right)$ and shown to lead to a classical Linear Programming problem that is amenable to sequential approximations, that are all $N$-Representable.

## Appendix

## A Operator Spaces

In the following the Fock space $\mathcal{H}_{\mathcal{F}}$ will be considered as the underlying Hilbert space on which the operators are defined and a few basic properties will be listed.

### A.1 Finite rank operators

An operator $X$ is a finite rank operator acting $\mathcal{H}_{\mathcal{F}}$ if

$$X = \sum_{1 \leq j \leq m < \infty} \alpha_j \left|\Phi_j\right\rangle\left\langle\Psi_j\right|, \tag{A1}$$

where $\left\{\Phi_j \middle| 1 \leq j \leq m\right\}$ and $\left\{\Psi_j \middle| 1 \leq j \leq m\right\}$ are orthonormal sets in $\mathcal{H}_{\mathcal{F}}$. The set of finite rank operators is denoted $\mathcal{B}_0(\mathcal{H}_{\mathcal{F}})$ and is not closed if $\mathcal{H}_{\mathcal{F}}$ is infinite dimensional.

### A.2 Bounded operators

The operator norm (also called the uniform norm) is defined as

$$\|X\|_{\mathcal{B}(\mathcal{H}_{\mathcal{F}})} = \sup_{|\Phi\rangle\in\mathcal{H}_F} \left\{ \left( \frac{\langle \Phi|\, X^{\dagger} X \Phi \rangle}{\langle \Phi|\, \Phi\rangle} \right)^{\frac{1}{2}} \right\} = \sup_{|\Phi\rangle\in\mathcal{H}_F} \left\{ \frac{\|X\Phi\|_{\mathcal{H}_F}}{\|\Phi\|_{\mathcal{H}_F}} \right\}, \tag{A2}$$

(where $\|\|_{\mathcal{H}_F}$ is the norm in $\mathcal{H}_F$), and the space of bounded operators acting on the Hilbert space $\mathcal{H}_{\mathcal{F}}$ as

$$\mathcal{B}(\mathcal{H}_{\mathcal{F}}) = \left\{ X \,\middle|\, \|X\|_{\mathcal{B}(\mathcal{H}_{\mathcal{F}})} < \infty \right\}. \tag{A3}$$

If one restricts attention to self adjoint operators $X = X^{\dagger}$ then it can be shown that

$$\|X\|_{\mathcal{B}(\mathcal{H}_{\mathcal{F}})} = \sup_{|\Phi\rangle\in\mathcal{H}_F} \left\{ \left| \frac{\langle \Phi|\, X\Phi\rangle}{\langle \Phi|\, \Phi\rangle} \right| \right\} \tag{A4}$$

and thus for positive operators, $X \geq 0$

$$\|X\|_{\mathcal{B}(\mathcal{H}_{\mathcal{F}})} = \sup_{|\Phi\rangle\in\mathcal{H}_F} \left\{ \frac{\langle \Phi|\, X\Phi\rangle}{\langle \Phi|\, \Phi\rangle} \right\}. \tag{A5}$$

The space $\mathcal{B}(\mathcal{H}_{\mathcal{F}})$ is closed in the operator norm topology.

### A.3 Compact operators

The space of compact operators, $\mathcal{C}(\mathcal{H}_{\mathcal{F}})$ , is the closed space produced by taking the closure of the set of finite rank operators with respect to the operator norm topology i.e. any compact operator can be expressed as

$$X = \lim_{m\to\infty} \sum_{1\leq j\leq m} \alpha_j \left|\Phi_j\right\rangle\left\langle\Psi_j\right|, \tag{A6}$$

in the sense that

$$\lim_{m\to\infty} \left\| X - \sum_{1\leq j\leq m} \alpha_j \left|\Phi_j\right\rangle\left\langle\Psi_j\right| \right\|_{\mathcal{B}(\mathcal{H}_{\mathcal{F}})} = 0. \tag{A7}$$

### A.4 Trace class operators

The trace class norm is defined as

$$\|X\|_1 = \mathrm{Tr}\left\{ \left( X^{\dagger} X \right)^{\frac{1}{2}} \right\} \tag{A8}$$

and the space of trace class operators acting on the Hilbert space $\mathcal{H}_{\mathcal{F}}$ as

$$\mathcal{B}_1\left(\mathcal{H}_{\mathcal{F}}\right) = \{X \,|\, \|X\|_1 < \infty\}. \tag{A9}$$

The space $\mathcal{B}_1\left(\mathcal{H}_{\mathcal{F}}\right)$ is closed with respect to the $\|\,\|_1$ norm, while the closure with respect to the $\|\,\|_{\mathcal{B}(\mathcal{H}_{\mathcal{F}})}$ norm produces $\mathcal{C}\left(\mathcal{H}_{\mathcal{F}}\right)$.

### A.5 Hilbert–Schmidt operators

The Hilbert–Schmidt norm is defined as

$$\|X\|_2 = (\mathrm{Tr}\{X^{\dagger}X\})^{\frac{1}{2}} \tag{A10}$$

and the space of Hilbert–Schmidt operators acting on the Hilbert space $\mathcal{H}_{\mathcal{F}}$ as

$$\mathcal{B}_2\left(\mathcal{H}_{\mathcal{F}}\right) = \{X \,|\, \|X\|_2 < \infty\}. \tag{A11}$$

The space $\mathcal{B}_2\left(\mathcal{H}_{\mathcal{F}}\right)$ is closed with respect to the $\|\,\|_2$ norm, while the closure with respect to $\|\,\|_{\mathcal{B}(\mathcal{H}_{\mathcal{F}})}$ norm produces $\mathcal{C}\left(\mathcal{H}_{\mathcal{F}}\right)$.

### A.6 Relationship between the spaces

The relationship between the spaces is

$$\mathcal{B}\left(\mathcal{H}_{\mathcal{F}}\right) \supseteq \mathcal{C}\left(\mathcal{H}_{\mathcal{F}}\right) \supseteq \mathcal{B}_2\left(\mathcal{H}_{\mathcal{F}}\right) \supseteq \mathcal{B}_1\left(\mathcal{H}_{\mathcal{F}}\right) \supseteq \mathcal{B}_0\left(\mathcal{H}_{\mathcal{F}}\right). \tag{A12}$$

The closure of $\mathcal{B}_0\left(\mathcal{H}_{\mathcal{F}}\right)$ (and thus of $\mathcal{C}\left(\mathcal{H}_{\mathcal{F}}\right)$, $\mathcal{B}_2\left(\mathcal{H}_{\mathcal{F}}\right)$ and $\mathcal{B}_1\left(\mathcal{H}_{\mathcal{F}}\right)$) with respect to the strong operator topology is $\mathcal{B}\left(\mathcal{H}_{\mathcal{F}}\right)$, where these limits can be defined as

$$X = \text{s-}\lim_{m\to\infty} X_m \Leftrightarrow \lim_{m\to\infty} \|(X - X_m)\,\Phi\|_{\mathcal{H}_{\mathcal{F}}} = 0 \quad \forall\,|\Phi\rangle \in \mathcal{H}_{\mathcal{F}}, \tag{A13}$$

in contrast to the uniform operator topology limits that are given by

$$\begin{aligned} X = \lim_{m\to\infty} X_m \Leftrightarrow \lim_{m\to\infty} \|(X - X_m)\|_{\mathcal{H}_{\mathcal{F}}} &= 0 \\ = \lim_{m\to\infty} \sup_{|\Phi\rangle\in\mathcal{H}_F} &\left\{\left(\frac{\left\langle \Phi\right|(X - X_m)^{\dagger}\left(X - X_m\right)\Phi\right\rangle}{\left\langle \Phi\right|\Phi\rangle}\right)^{\frac{1}{2}}\right\}. \end{aligned} \tag{A14}$$

If the dimension of $\mathcal{H}_{\mathcal{F}}$ is finite all of these spaces are identical and closed in all of the preceding norms and topologies.

## B Projectors

A general element of $\Lambda_2$ can be expanded as

$$\lambda = \sum_{1\le j,k\le r} \lambda_{1jk} a_j^\dagger a_k + \sum_{\substack{1\le j<k\le r\\ 1\le l<m\le r}} \lambda_{2jklm} a_j^\dagger a_k^\dagger a_m a_l \tag{B1}$$

and the condition that it is a projector i.e. idempotent is that

$$\lambda = \lambda^2, \tag{B2}$$

which implies

$$\lambda = \lambda^\dagger \quad \text{and} \quad \lambda \ge 0. \tag{B3}$$

In a $c^*$-algebra

$$\left\| X^\dagger X \right\| = \|X\|^2 \tag{B4}$$

The idempotency condition Eq. B2 implies that

$$\left\| \lambda^2 \right\| = \|\lambda\| \tag{B5}$$

and the $c^*$-norm property Eq. B4

$$\left\| \lambda^2 \right\| = \|\lambda\|^2 \tag{B6}$$

gives

$$\|\lambda\|^2 = \|\lambda\| \tag{B7}$$

and thus

$$\|\lambda\| = 1. \tag{B8}$$

### B.1 One electron case

We first consider the case $\lambda_2 = 0$ then

$$\lambda_1 = \lambda_1^2 \tag{B9}$$

and noting that $\lambda_1$ must be self adjoint and positive one has

$$\lambda = \lambda_1 = \sum_{1\le j,k\le\infty} \lambda_{1jk} a_j^\dagger a_k = \sum_{\substack{1\le j,k\le r\\ 1\le l\le r}} u_{jl}\beta_l \bar{u}_{kl} a_j^\dagger a_k = \sum_{1\le l\le r} \beta_l b_l^\dagger b_l, \tag{B10}$$

where

$$1 \ge \beta_l \ge 0;\ 1 \le j \le r \tag{B11a}$$
$$b_l^\dagger = \sum_{1\le j\le r} a_j^\dagger u_{jl} \tag{B11b}$$
$$b_l^\dagger \left|\phi\right\rangle = \left|\psi_l\right\rangle \tag{B11c}$$
$$\mathbb{U}_1^\dagger \mathbb{U}_1 = \mathbb{U}_1 \mathbb{U}_1^\dagger = \mathbb{I}_r, \tag{B11d}$$

where $\mathbb{U}_1$ is the matrix composed of the matrix elements $\left\{u_{jk}\middle| 1 \le j,k \le r\right\}$. The condition Eq. B9 becomes

$$\sum_{1\le l\le r} \beta_l b_l^\dagger b_l = \sum_{1\le l\le r} \beta_l^2 b_l^\dagger b_l + 2\sum_{1\le l_1<l_2\le r} \beta_{l_1}\beta_{l_2} b_{l_1}^\dagger b_{l_1} b_{l_2}^\dagger b_{l_2}, \tag{B12}$$

which can be rewritten as

$$\sum_{1\le l\le r} \{\beta_l (1-\beta_l)\} b_l^\dagger b_l = 2\sum_{1\le l_1<l_2\le r} \beta_{l_1}\beta_{l_2} b_{l_1}^\dagger b_{l_2}^\dagger b_{l_2} b_{l_1}. \tag{B13}$$

This equality must be true on all vectors in $\mathcal{H}_{\mathcal{F}}$ in particular on $\left|\psi_\kappa\right\rangle \in \mathcal{H}^1$, $1 \le \kappa \le r$, i.e.

$$\sum_{1\le l\le r} \{\beta_l (1-\beta_l)\} b_l^\dagger b_l \left|\psi_\kappa\right\rangle = 2\sum_{1\le l_1<l_2\le r} \beta_{l_1}\beta_{l_2} b_{l_1}^\dagger b_{l_2}^\dagger b_{l_2} b_{l_1} \left|\psi_\kappa\right\rangle, \tag{B14}$$

which gives

$$\beta_\kappa (1-\beta_\kappa) \left|\psi_\kappa\right\rangle = 0, \quad 1 \le \kappa \le r \tag{B15}$$

i.e.

$$\beta_\kappa = 0 \text{ or } \beta_\kappa = 1, \quad 1 \le \kappa \le r. \tag{B16}$$

One can see that $\beta_\kappa = 1$ for only one value of $\kappa \in \{1,\ldots,r\}$, for let $\{n_1,\ldots,n_{r'}\}$ be a subset of $\{1,\ldots,r\}$ and

$$\lambda_1 = \sum_{\substack{1\le\nu\le\kappa\le r\\ \sigma_\nu\in\{1,\ldots,r\}}} b_{\sigma_\nu}^\dagger b_{\sigma_\nu} \tag{B17}$$

then

$$\lambda_1^2 = \sum_{\sigma\in\{1,\ldots,r\}} b_\sigma^\dagger b_\sigma + \sum_{\sigma,\sigma'\in\{1,\ldots,r\}} b_\sigma^\dagger b_{\sigma'}^\dagger b_{\sigma'} b_\sigma = \lambda_1 = \sum_{\sigma\in\{1,\ldots,r\}} b_\sigma^\dagger b_\sigma \quad \text{(B18)}$$

thus

$$\sum_{\sigma,\sigma'\in\{1,\ldots,r\}} b_\sigma^\dagger b_{\sigma'}^\dagger b_{\sigma'} b_\sigma = 0, \quad \text{(B19)}$$

which is only possible if $r' = 1$. Thus if $\lambda_1$ is a projector it must be of the form

$$\lambda_1 = b^\dagger b. \quad \text{(B20)}$$

B.2 Two electron case

We consider the case $\lambda_1 = 0$ then

$$\lambda_2 = \lambda_2^2 \quad \text{(B21)}$$

and

$$\lambda = \lambda_2 = \sum_{\substack{1\le j_1<j_2\le r\\ 1\le k_1<k_2\le r}} \lambda_{2\,j_1 j_2 k_1 k_2} a_{j_1}^\dagger a_{j_2}^\dagger a_{k_2} a_{k_1} = \sum_{\substack{1\le j_1<j_2\le r\\ 1\le k_1<k_2\le r\\ 1\le l\le\binom{r}{2}}} u_{j_1 j_2 l}\beta_l \bar{u}_{l k_1 k_2} a_{j_1}^\dagger a_{j_2}^\dagger a_{k_2} a_{k_1}$$
$$= \sum_{1\le l\le\binom{r}{2}} \beta_l g_l^\dagger g_l, \quad \text{(B22)}$$

where the matrix that diagonalizes the matrix

$$\lambda_2 \equiv \left\{ \lambda_{2\,j_1 j_2 k_1 k_2} \middle| 1 \le j_1 < j_2 \le r; 1 \le k_1 < k_2 \le r \right\} \quad \text{(B23)}$$

is unitary i.e.

$$\mathbb{U}_2^\dagger \mathbb{U}_2 = \mathbb{U}_2 \mathbb{U}_2^\dagger = \mathbb{I}_{\binom{r}{2}}, \quad \text{(B24)}$$

so that

$$\lambda_2 = \mathbb{U}_2 \begin{pmatrix} \beta_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \beta_{\binom{r}{2}} \end{pmatrix} \mathbb{U}_2^\dagger. \quad \text{(B25)}$$

The geminal creators $\left\{ g_l^\dagger \middle| 1 \leq l \leq \binom{r}{2} \right\}$, geminal coefficients $\left\{ g_{lj_1j_2} \middle| 1 \leq j_1 < j_2 \leq r \right\}$ and the geminal coefficient matrices $\mathbb{G}_l$ have the properties

$$g_l^\dagger = \sum_{1 \leq j_1 < j_2 \leq r} g_{lj_1j_2} a_{j_1}^\dagger a_{j_2}^\dagger = \frac{1}{2} \sum_{1 \leq j_1, j_2 \leq r} g_{lj_1j_2} a_{j_1}^\dagger a_{j_2}^\dagger; \tag{B26a}$$

$$\mathbb{G}_{lj_1j_2} = g_{lj_1j_2} = -g_{lj_2j_1} = u_{j_1j_2l} \tag{B26b}$$

$$g_l^\dagger |\phi\rangle = |g_l\rangle \;; \quad 1 \leq l \leq \binom{r}{2} \tag{B26c}$$

$$\langle g_{l_1} | g_{l_2} \rangle = \delta_{l_1l_2}; \quad 1 \leq l_1, l_2 \leq \binom{r}{2} \tag{B26d}$$

$$\mathrm{Tr}\left\{ \mathbb{G}_{l_1}^\dagger \mathbb{G}_{l_2} \right\} = 2\delta_{l_1l_2}; \quad 1 \leq l_1, l_2 \leq \binom{r}{2} \tag{B26e}$$

$$\mathbb{G}_l = -\mathbb{G}_l^t; \quad 1 \leq l \leq \binom{r}{2}. \tag{B26f}$$

The values of the $\beta_l$'s in Eq. B22 are restricted by

$$1 \geq \beta_l \geq 0; 1 \leq l \leq \binom{r}{2} \tag{B27}$$

as the projection of $\lambda_2$ on $\mathcal{H}^2$ is given by

$$P_{\mathcal{H}^2} \lambda_2 P_{\mathcal{H}^2} = \sum_{1 \leq l \leq \binom{r}{2}} \beta_l |g_l\rangle \langle g_l| \,, \tag{B28}$$

where $\lambda_2$ is the second quantization of $P_{\mathcal{H}^2} \lambda_2 P_{\mathcal{H}^2}$ i.e.

$$\lambda_2 = \Gamma\left( P_{\mathcal{H}^2} \lambda_2 P_{\mathcal{H}^2} \right), \tag{B29}$$

thus

$$\lambda_2 \geq 0 \Rightarrow P_{\mathcal{H}^2} \lambda_2 P_{\mathcal{H}^2} \geq 0 \tag{B30}$$

and

$$\lambda_2 - P_{\mathcal{H}^2} \lambda_2 P_{\mathcal{H}^2} \geq 0, \tag{B31}$$

as $\|\lambda_2\| = 1$ ($\lambda_2$ is a projector) the eigenvalues of $P_{\mathcal{H}^2} \lambda_2 P_{\mathcal{H}^2} \in [0, 1]$ .

*B.2.1 Two electron operator idempotency condition*

**Lemma 1** *If* $\lambda_2$ *is a projector then* $\lambda_2 = \sum_{1 \leq l \leq \binom{r}{2}} \beta_l g_l^\dagger g_l$, *where* $\beta_l = 1$ *or 0.*

*Proof* Using the expansion Eq. B22 of the operator $\lambda_2$ the idempotency condition Eq. B21 becomes

$$\sum_{1\leq l\leq\binom{r}{2}} \beta_l g_l^\dagger g_l = \sum_{1\leq l_1,l_2\leq\binom{r}{2}} \beta_{l_1}\beta_{l_2} g_{l_1}^\dagger g_{l_1} g_{l_2}^\dagger g_{l_2} \tag{B32}$$

and one must compare the left hand side of Eq. B32 to the right hand side. In order to do this one needs to bring the RHS of Eq. B32 to normal form by sequentially using the canonical anti commutation relationships. The first step produces

$$\begin{aligned}\sum_{1\leq l_1,l_2\leq\binom{r}{2}} &\beta_{l_1}\beta_{l_2} g_{l_1}^\dagger g_{l_1} g_{l_2}^\dagger g_{l_2} \\ &= \sum_{1\leq l_1,l_2\leq\binom{r}{2}} \beta_{l_1}\beta_{l_2} \left\{g_{l_1}^\dagger \left[g_{l_1}, g_{l_2}^\dagger\right] g_{l_2} + g_{l_1}^\dagger g_{l_2}^\dagger g_{l_1} g_{l_2}\right\}.\end{aligned} \tag{B33}$$

which can be developed by noting that

$$\begin{aligned}\left[g_{l_1}, g_{l_2}^\dagger\right] &= \frac{1}{4}\sum_{\substack{1\leq j_1,j_2\leq r\\1\leq k_1,k_2\leq r}} \bar{g}_{l_1 j_1 j_2} g_{l_2 k_1 k_2}\left[a_{j_2}a_{j_1}, a_{k_1}^\dagger a_{k_2}^\dagger\right]\\ &= -\frac{1}{4}\sum_{\substack{1\leq j_1,j_2\leq r\\1\leq k_1,k_2\leq r}} \bar{g}_{l_1 j_1 j_2} g_{l_2 k_1 k_2}\left[a_{k_1}^\dagger a_{k_2}^\dagger, a_{j_2}a_{j_1}\right],\end{aligned} \tag{B34}$$

and (“Appendix B.2.1”)

$$\begin{aligned}\left[a_{k_1}^\dagger a_{k_2}^\dagger, a_{j_2}a_{j_1}\right] = I_{\mathcal{H}_\mathcal{F}}\delta_{j_2k_1}\delta_{j_1k_2} - I_{\mathcal{H}_\mathcal{F}}\delta_{j_2k_2}\delta_{j_1k_1} + a_{k_2}^\dagger a_{j_2}\delta_{j_1k_1}\\ -a_{k_1}^\dagger a_{j_2}\delta_{j_1k_2} - a_{k_2}^\dagger a_{j_1}\delta_{j_2k_1} + a_{k_1}^\dagger a_{j_1}\delta_{j_2k_2}\end{aligned} \tag{B35}$$

to give

$$\begin{aligned}\left[g_{l_1}, g_{l_2}^\dagger\right] &= -\frac{1}{4}\sum_{\substack{1\leq j_1,j_2\leq r\\1\leq k_1,k_2\leq r}} \bar{g}_{l_1 j_1 j_2} g_{l_2 k_1 k_2}\left\{I_{\mathcal{H}_\mathcal{F}}\delta_{j_2k_1}\delta_{j_1k_2} - I_{\mathcal{H}_\mathcal{F}}\delta_{j_2k_2}\delta_{j_1k_1}\right.\\ &\quad \left. a_{k_2}^\dagger a_{j_2}\delta_{j_1k_1} - a_{k_1}^\dagger a_{j_2}\delta_{j_1k_2} - a_{k_2}^\dagger a_{j_1}\delta_{j_2k_1} + a_{k_1}^\dagger a_{j_1}\delta_{j_2k_2}\right\},\\ &= \frac{1}{2}\sum_{1\leq j_1,j_2\leq r} \bar{g}_{l_1 j_1 j_2} g_{l_2 j_1 j_2}\\ &\quad -\frac{1}{4}\sum_{\substack{1\leq j,j_2\leq r\\1\leq k_2\leq r}}\left\{\bar{g}_{l_1 j j_2} g_{l_2 j k_2} - \bar{g}_{l_1 j j_2} g_{l_2 k_2 j} - \bar{g}_{l_1 j_2 j} g_{l_2 j k_2} + \bar{g}_{l_1 j_2 j} g_{l_2 k_2 j}\right\} a_{k_2}^\dagger a_{j_2},\end{aligned} \tag{B36}$$

and after using $g_{ljk} = -g_{lkj}$

$$\left[g_{l_1}, g_{l_2}^{\dagger}\right] = \delta_{l_1 l_2} + \sum_{1 \le j,k \le r} \bar{g}_{l_1 jj} g_{l_2 jk} a_k^{\dagger} a_j = \delta_{l_1 l_2} - \sum_{1 \le j_2, k_2 \le r} \left(\mathbb{G}_{l_1}^{\dagger} \mathbb{G}_{l_2}\right)_{jk} a_k^{\dagger} a_j. \tag{B37}$$

The idempotency condition then becomes

$$\begin{aligned}\sum_{1 \le l \le \binom{r}{2}} \beta_l g_l^{\dagger} g_l &= \sum_{1 \le l_1, l_2 \le \binom{r}{2}} \beta_{l_1} \beta_{l_2} g_{l_1}^{\dagger} g_{l_1} g_{l_2}^{\dagger} g_{l_2} \\ &= \sum_{1 \le l_1, l_2 \le \binom{r}{2}} \beta_{l_1} \beta_{l_2} \left\{ g_{l_1}^{\dagger} \left\{ \delta_{l_1 l_2} - \sum_{1 \le j_2, k_2 \le r} \left(\mathbb{G}_{l_1}^{\dagger} \mathbb{G}_{l_2}\right)_{j_2 k_2} a_{k_2}^{\dagger} a_{j_2} \right\} \right. \\ &\qquad \left. \times\, g_{l_2} + g_{l_1}^{\dagger} g_{l_2}^{\dagger} g_{l_1} g_{l_2} \right\},\end{aligned} \tag{B38}$$

which simplifies to

$$\begin{aligned}\sum_{1 \le l \le \binom{r}{2}} \beta_l g_l^{\dagger} g_l &= \sum_{1 \le l \le \binom{r}{2}} \beta_l^2 g_l^{\dagger} g_l \\ &\quad - \sum_{1 \le l_1, l_2 \le \binom{r}{2}} \beta_{l_1} \beta_{l_2} \left\{ \sum_{1 \le j_2, k_2 \le r} \left(\mathbb{G}_{l_1}^{\dagger} \mathbb{G}_{l_2}\right)_{j_2 k_2} g_{l_1}^{\dagger} a_{k_2}^{\dagger} a_{j_2} g_{l_2} + g_{l_1}^{\dagger} g_{l_2}^{\dagger} g_{l_1} g_{l_2} \right\} \\ &= \sum_{1 \le l \le \binom{r}{2}} \beta_l^2 g_l^{\dagger} g_l - \sum_{1 \le l_1, l_2 \le \binom{r}{2}} \beta_{l_1} \beta_{l_2} \sum_{1 \le j_2, k_2 \le r} \left(\mathbb{G}_{l_1}^{\dagger} \mathbb{G}_{l_2}\right)_{j_2 k_2} g_{l_1}^{\dagger} a_{k_2}^{\dagger} a_{j_2} g_{l_2} \\ &\quad - \sum_{1 \le l_1, l_2 \le \binom{r}{2}} \beta_{l_1} \beta_{l_2} g_{l_1}^{\dagger} g_{l_2}^{\dagger} g_{l_1} g_{l_2}.\end{aligned} \tag{B39}$$

The operator equality in Eq. B39 must be true on all vectors thus in particular

$$\begin{aligned}&\sum_{1 \le l \le \binom{r}{2}} \beta_l g_l^{\dagger} g_l \left|g_p\right\rangle = \sum_{1 \le l \le \binom{r}{2}} \beta_l^2 g_l^{\dagger} g_l \left|g_p\right\rangle \Longleftrightarrow \beta_p \left(\beta_p - 1\right) = 0; \\ &1 \le p \le \binom{r}{2}\end{aligned} \tag{B40}$$

leading to

$$\lambda_2 = \sum_{\substack{1 \le \nu \le \kappa \le \binom{r}{2} \\ \sigma_\nu \in \left\{1, \ldots, \binom{r}{2}\right\}}} g_{\sigma_\nu}^{\dagger} g_{\sigma_\nu}; \quad \sigma_\nu \ne \sigma_{\nu'} \quad \text{unless } \nu = \nu', \tag{B41}$$

where $\kappa$ is the number of non zero $\beta' s$. □

**Lemma 2** *If $\lambda_2$ is a projector then $\lambda_2 = g^\dagger g$, where $g^\dagger$ creates a normalized geminal.*

*Proof* As $\lambda_2$ is a projection operator its eigenvalues are 1 or 0 and as $[\lambda_2, \mathcal{N}_1] = 0$ its eigenvectors can be chosen to simultaneously diagonalize the number operator $\mathcal{N}_1$.

In the finite dimensional case, i.e. $r < \infty$, the subspace $\mathcal{H}^r$ is one dimensional and is spanned by a single normalized r-fold antisymmetrized product, $|\varphi_1 \ldots \varphi_r\rangle$, formed from *any* orthonormal basis, $\left\{\varphi_j \middle| 1 \le j \le r\right\}$ of $\mathcal{H}^1$, i.e.

$$|\varphi_1 \ldots \varphi_r\rangle \overset{\text{up to a phase factor}}{=} \left|\varphi'_1 \ldots \varphi'_r\right\rangle, \tag{B42}$$

where $\left\{\varphi_j \middle| 1 \le j \le r\right\}$ and $\left\{\varphi'_j \middle| 1 \le j \le r\right\}$ are arbitrary orthonormal bases of $\mathcal{H}^1$. Thus any vector in $\mathcal{H}^r$ is an eigenvector of $\lambda_2$, as $\lambda_2 : \mathcal{H}^r \to \mathcal{H}^r$.

Any geminal creator $g_l^\dagger$ can be expressed in canonical form as [26,27]

$$g_l^\dagger = \sum_{1\le j\le s} c_{lj} a_{lj}^\dagger a_{lj+s}^\dagger; \quad c_{lj} \ge 0, 1 \le j \le s, \tag{B43}$$

where

$$\sum_{1\le j\le s} c_{lj}^2 = 1 \tag{B44}$$

and the canonical general spin orbitals of $|g_l\rangle = g_l^\dagger\,|\phi\rangle$ are produced by

$$a_{lj}^\dagger\,|\phi\rangle = \left|\varphi_{lj}\right\rangle. \tag{B45}$$

Hence

$$g_l^\dagger g_l = \sum_{1\le j,k\le s} c_{lj} c_{lk} a_{lj}^\dagger a_{lj+s}^\dagger a_{lk+s} a_{lk} \tag{B46}$$

and $\lambda_2$ can be expanded (noting that $\beta_l = 1$ or $0$, $1 \le l \le \binom{r}{2}$) as

$$\langle\varphi_1 \ldots \varphi_r\,|\lambda_2 \varphi_1 \ldots \varphi_r\,\rangle = \sum_{1\le l\le\binom{r}{2}} \beta_l \left\langle\varphi_{l1} \ldots \varphi_{lr}\,\middle|g_l^\dagger g_l \varphi_{l1} \ldots \varphi_{lr}\right\rangle \tag{B47}$$

$$= \sum_{\substack{1\le j,k\le s\\ 1\le l\le\binom{r}{2}}} \beta_l c_{lj} c_{lk} \left\langle\varphi_{l1} \ldots \varphi_{lr}\,\middle|a_{lj}^\dagger a_{lj+s}^\dagger a_{lk+s} a_{lk} \varphi_{l1} \ldots \varphi_{lr}\right\rangle \tag{B48}$$

$$= \sum_{\substack{1\le j\le s\\ 1\le l\le\binom{r}{2}}} \beta_l c_{lj}^2 = \sum_{1\le l\le\binom{r}{2}} \beta_l. \tag{B49}$$

The vector $|\varphi_1 \ldots \varphi_r\rangle$ is an eigenvector of $\lambda_2$ with eigenvalue 1 (as $\lambda_2$ is a projector) thus

$$\sum_{1 \le l \le \binom{r}{2}} \beta_l = 1, \tag{B50}$$

as $\beta_l = 1$ or 0, $1 \le l \le \binom{r}{2}$ only one $\beta_l$ can be non zero and $\lambda = g^\dagger g$. □

Thus one can prove the following theorem:

**Theorem 3** $\lambda_2 \in \mathcal{B}(\mathcal{H}_\mathcal{F})_2$ *is a projector if only if it can be expressed in the form* $\lambda_2 = a^\dagger b^\dagger ba$, *where* $a^\dagger$ *and* $b^\dagger$ *create normalized orthogonal vectors in* $\mathcal{H}^1$.

*Proof* Using the two preceding lemmas one has that if $\lambda_2$ is a two electron projector

$$\lambda_2 = g^\dagger g$$

and thus

$$\lambda_2^2 = g^\dagger g g^\dagger g. \tag{B51}$$

Using the canonical expansion of the geminal one can expand Eq. B51 as

$$g^\dagger g g^\dagger g = \sum_{1 \le j_1, j_2, j_3, j_4 \le s} a^\dagger_{j_1} a^\dagger_{j_{1+s}} a_{j_2} a_{j_{2+s}} a^\dagger_{j_3} a^\dagger_{j_{3+s}} a_{j_4} a_{j_{4+s}} c_{j_1} c_{j_2} c_{j_3} c_{j_4}. \tag{B52}$$

and bring Eq. B52 to normal form by observing that

$$\begin{aligned}
&a_{j_2} a_{j_{2+s}} a^\dagger_{j_3} a^\dagger_{j_{3+s}} \\
&\quad = \delta_{j_2 j_{3+s}} \delta_{j_{2+s} j_3} - \delta_{j_2 j_3} \delta_{j_{2+s} j_{3+s}} - a^\dagger_{j_{3+s}} a_{j_2} \delta_{j_{2+s} j_3} \\
&\qquad + a^\dagger_{j_3} a_{j_2} \delta_{j_{2+s} j_{3+s}} + a^\dagger_{j_{3+s}} a_{j_{2+s}} \delta_{j_2 j_3} - a^\dagger_{j_3} a_{j_{2+s}} \delta_{j_2 j_{3+s}} + a^\dagger_{j_3} a^\dagger_{j_{3+s}} a_{j_{2+s}} a_{j_2} \\
&\quad = -I \delta_{j_2 j_3} + a^\dagger_{j_3} a_{j_2} \delta_{j_2 j_3} + a^\dagger_{j_3} a_{j_2} \delta_{j_2 j_3} + a^\dagger_{j_3} a^\dagger_{j_{3+s}} a_{j_{2+s}} a_{j_2}
\end{aligned} \tag{B53}$$

and obtaining

$$\begin{aligned}
g^\dagger g g^\dagger g &= \sum_{1 \le j_1, j_2, j_3, j_4 \le s} a^\dagger_{j_1} a^\dagger_{j_{1+s}} \Big( -\delta_{j_2 j_3} + a^\dagger_{j_3} a_{j_2} \delta_{j_2 j_3} + a^\dagger_{j_{3+s}} a_{j_{2+s}} \delta_{j_2 j_3} \\
&\qquad + a^\dagger_{j_3} a^\dagger_{j_{3+s}} a_{j_{2+s}} a_{j_2} \Big) \times a_{j_4} a_{j_{4+s}} c_{j_1} c_{j_2} c_{j_3} c_{j_4} \\
&= \sum_{1 \le j_1, j_4 \le s} a^\dagger_{j_1} a^\dagger_{j_{1+s}} a_{j_{4+s}} a_{j_4} c_{j_1} c_{j_4} \, \|g\|^2_{\mathcal{H}^2} \\
&\quad + \sum_{1 \le j_1, j_2, j_4 \le s} c_{j_1} a^\dagger_{j_1} a^\dagger_{j_{1+s}} n_{j_2} \left( a^\dagger_{j_2} a_{j_2} + a^\dagger_{j_{2+s}} a_{j_{2+s}} \right) a_{j_4} a_{j_{4+s}} c_{j_4} \\
&\quad + \sum_{1 \le j_1, j_2, j_3, j_4 \le s} a^\dagger_{j_1} a^\dagger_{j_{1+s}} a^\dagger_{j_3} a^\dagger_{j_{3+s}} a_{j_{2+s}} a_{j_2} a_{j_4} a_{j_{4+s}} c_{j_1} c_{j_2} c_{j_3} c_{j_4},
\end{aligned} \tag{B54}$$

where $n_j = a_j^\dagger a_j$. The difference between $\lambda_2^2$ and $\lambda_2$ can then be expressed as

$$\Xi = g^\dagger g g^\dagger g - g^\dagger g = \sum_{1\le j_1, j_2, j_4 \le s} c_{j_1} a_{j_1}^\dagger a_{j_{1+s}}^\dagger n_{j_2} \left( a_{j_2}^\dagger a_{j_2} + a_{j_2+s}^\dagger a_{j_2+s} \right) a_{j_4} a_{j_{4+s}} c_{j_4} + \sum_{1\le j_1, j_2, j_3, j_4 \le s} a_{j_1}^\dagger a_{j_{1+s}}^\dagger a_{j_3}^\dagger a_{j_{3+s}}^\dagger a_{j_{2+s}} a_{j_2} a_{j_4} a_{j_{4+s}} c_{j_1} c_{j_2} c_{j_3} c_{j_4} \tag{B55}$$

and one can note that

$$\Xi = g^\dagger g g^\dagger g - g^\dagger g = 0 \quad \Updownarrow \quad P_{\mathcal{H}^m} \Xi P_{\mathcal{H}^m} = 0 \forall m. \tag{B56}$$

Thus in particular

$$\left\langle \Phi \left| \sum_{1\le j_1, j_2, j_4 \le s} c_{j_1} a_{j_1}^\dagger a_{j_{1+s}}^\dagger n_{j_2} \left( a_{j_2}^\dagger a_{j_2} + a_{j_2+s}^\dagger a_{j_2+s} \right) a_{j_4} a_{j_{4+s}} c_{j_4} \ \Psi \right. \right\rangle = 0 \quad \forall \Phi, \Psi \in \mathcal{H}^3. \tag{B57}$$

Letting

$$|\Phi\rangle = |\Psi\rangle = \left| \varphi_j \varphi_{j+s} \varphi_k \right\rangle \tag{B58}$$

one obtains

$$\begin{aligned} 0 &= \left\langle \varphi_j \varphi_{j+s} \varphi_k \left| \sum_{1\le j_1, j_2, j_4 \le s} c_{j_1} a_{j_1}^\dagger a_{j_{1+s}}^\dagger n_{j_2} \left( a_{j_2}^\dagger a_{j_2} + a_{j_2+s}^\dagger a_{j_2+s} \right) a_{j_4} a_{j_{4+s}} c_{j_4} \varphi_j \varphi_{j+s} \varphi_k \right. \right\rangle \\ &= \sum_{1\le j_1, j_2, j_4 \le s} c_{j_1} c_{j_4} n_{j_2} \left\{ \left\langle \varphi_j \varphi_{j+s} \varphi_k \left| a_{j_1}^\dagger a_{j_{1+s}}^\dagger a_{j_2}^\dagger a_{j_2} a_{j_4} a_{j_{4+s}} \varphi_j \varphi_{j+s} \varphi_k \right. \right\rangle \right. \\ &\quad + \left. \left\langle \varphi_j \varphi_{j+s} \varphi_k \left| a_{j_1}^\dagger a_{j_{1+s}}^\dagger a_{j_2+s}^\dagger a_{j_2+s} a_{j_4} a_{j_{4+s}} \varphi_j \varphi_{j+s} \varphi_k \right. \right\rangle \right\} = n_j n_k \left( 1 - \delta_{jk} - \delta_{(j+s)k} \right). \end{aligned} \tag{B59}$$

Thus

$$n_j n_{|k|} = 0 \quad j \ne k \,;\, 1 \le j \le s, 1 \le k \le 2s, \tag{B60}$$

i.e.

$$\begin{aligned} n_1 n_2 = n_1 n_3 = \cdots = n_1 n_s = 0 \\ n_2 n_1 = n_2 n_3 = \cdots = n_2 n_s = 0, \end{aligned} \tag{B61}$$

where

$$|k| = \begin{cases} k & \text{if } k \leq s \\ k - s & \text{if } k > s \end{cases}. \tag{B62}$$

One can then see from Eq. B61 that all but one of the occupation numbers must be zero and the one that isn't must equal one, thus the rank of the geminal creator $g^\dagger$ must be 1. □

Mixed case

The general case concerns projectors of the form

$$\lambda = \lambda_1 + \lambda_2, \tag{B63}$$

which is handled by considering:

*Q projectors*

Using the particle-hole transformation

$$a^\dagger \to a \tag{B64}$$

of the Fock algebra and the preceding lemmas and theorem one can see that all projectors formed from two electron hole operators must be of the form

$$A^\dagger A, \tag{B65}$$

where

$$A = b^\dagger a^\dagger, \tag{B66}$$

i.e.

$$A^\dagger A = abb^\dagger a^\dagger, \tag{B67}$$

which is a projector as

$$\begin{aligned}\left(abb^\dagger a^\dagger\right)^2 &= abb^\dagger a^\dagger abb^\dagger a^\dagger = abb^\dagger \left(1 - aa^\dagger\right) bb^\dagger a^\dagger \\ &= abb^\dagger bb^\dagger a^\dagger - abb^\dagger aa^\dagger bb^\dagger a^\dagger = ab \left(1 - bb^\dagger\right) b^\dagger a^\dagger = abb^\dagger a^\dagger.\end{aligned} \tag{B68}$$

Noting that

$$abb^\dagger a^\dagger = I_{\mathcal{H}_\mathcal{F}} - a^\dagger a - b^\dagger b + a^\dagger b^\dagger ba = I_{\mathcal{H}_\mathcal{F}} - \Lambda, \tag{B69}$$

where

$$\Lambda = a^{\dagger}a + b^{\dagger}b - a^{\dagger}b^{\dagger}ba \tag{B70}$$

one has

$$I_{\mathcal{H}_{\mathcal{F}}} - \Lambda = \left(I_{\mathcal{H}_{\mathcal{F}}} - \Lambda\right)^2 = I_{\mathcal{H}_{\mathcal{F}}} - 2\Lambda + \Lambda^2, \tag{B71}$$

which shows that

$$\Lambda^2 = \Lambda, \tag{B72}$$

i.e.

$$\Lambda = a^{\dagger}a + b^{\dagger}b - a^{\dagger}b^{\dagger}ba \tag{B73}$$

are projectors that belong to $\mathcal{B}\left(\mathcal{H}_{\mathcal{F}}\right)_1 \oplus \mathcal{B}\left(\mathcal{H}_{\mathcal{F}}\right)_2$ and lead to the generalized Q-Conditions.

*G projectors*

The generalized G-Condition is based on the product

$$A^{\dagger}A, \tag{B74}$$

where

$$A = b^{\dagger}a, \tag{B75}$$

i.e.

$$\begin{aligned} A^{\dagger}A &= a^{\dagger}bb^{\dagger}a = a^{\dagger}\left(I_{\mathcal{H}_{\mathcal{F}}} - b^{\dagger}a\right)a = a^{\dagger}a - a^{\dagger}b^{\dagger}ba = n_a - n_a n_b \\ &= n_a\left(1 - n_b\right). \end{aligned} \tag{B76}$$

The operator $a^{\dagger}a - a^{\dagger}b^{\dagger}ba$ is a projector as

$$n_a\left(1 - n_b\right)n_a\left(1 - n_b\right) = n_a\left(1 - n_b\right)^2 = n_a\left(1 - 2n_b + n_b\right) = n_a\left(1 - n_b\right) \tag{B77}$$

and

$$a^{\dagger}a - a^{\dagger}b^{\dagger}ba \in \Lambda_2. \tag{B78}$$

## Two electron commutation relationships

The commutator

$$\left[a^{\dagger}_{k_1}a^{\dagger}_{k_2}, a_{j_2}a_{j_1}\right] \tag{C1}$$

is evaluated by bringing $a_{j_4}a_{j_3}a^{\dagger}_{j_1}a^{\dagger}_{j_2}$ to normal form as

$$\begin{aligned}
a_{j_2}a_{j_1}a^{\dagger}_{k_1}a^{\dagger}_{k_2} &= a_{j_2}\left(\delta_{j_1k_1} - a^{\dagger}_{k_1}a_{j_1}\right)a^{\dagger}_{k_2} = a_{j_2}a^{\dagger}_{k_2}\delta_{j_1k_1} - a_{j_2}a^{\dagger}_{k_1}a_{j_1}a^{\dagger}_{k_2}\\
&= \left(\delta_{j_2k_2} - a^{\dagger}_{k_2}a_{j_2}\right)\delta_{j_1k_1} - \left(\delta_{j_2k_1} - a^{\dagger}_{k_1}a_{j_2}\right)\left(\delta_{j_1k_2} - a^{\dagger}_{k_2}a_{j_1}\right)\\
&= \delta_{j_2k_2}\delta_{j_1k_1} - a^{\dagger}_{k_2}a_{j_2}\delta_{j_1k_1} - \delta_{j_2k_1}\delta_{j_1k_2} + a^{\dagger}_{k_1}a_{j_2}\delta_{j_1k_2} + a^{\dagger}_{k_2}a_{j_1}\delta_{j_2k_1}\\
&\quad - a^{\dagger}_{k_1}a_{j_2}a^{\dagger}_{k_2}a_{j_1}\\
&= \delta_{j_2k_2}\delta_{j_1k_1} - \delta_{j_2k_1}\delta_{j_1k_2} - a^{\dagger}_{k_2}a_{j_2}\delta_{j_1k_1} + a^{\dagger}_{k_1}a_{j_2}\delta_{j_1k_2} + a^{\dagger}_{k_2}a_{j_1}\delta_{j_2k_1}\\
&\quad - a^{\dagger}_{k_1}\left(\delta_{j_2k_2} - a^{\dagger}_{k_2}a_{j_2}\right)a_{j_1}\\
&= \delta_{j_2k_2}\delta_{j_1k_1} - \delta_{j_2k_1}\delta_{j_1k_2} - a^{\dagger}_{k_2}a_{j_2}\delta_{j_1k_1} + a^{\dagger}_{k_1}a_{j_2}\delta_{j_1k_2} + a^{\dagger}_{k_2}a_{j_1}\delta_{j_2k_1}\\
&\quad - a^{\dagger}_{k_1}a_{j_1}\delta_{j_2k_2} + a^{\dagger}_{k_1}a^{\dagger}_{k_2}a_{j_2}a_{j_1}
\end{aligned} \tag{C2}$$

giving

$$\begin{aligned}
a_{j_2}a_{j_1}a^{\dagger}_{k_1}a^{\dagger}_{k_2} &= I_{\mathcal{H}_{\mathcal{F}}}\delta_{j_2k_2}\delta_{j_1k_1} - I_{\mathcal{H}_{\mathcal{F}}}\delta_{j_2k_1}\delta_{j_1k_2} - a^{\dagger}_{k_2}a_{j_2}\delta_{j_1k_1}\\
&\quad + a^{\dagger}_{k_1}a_{j_2}\delta_{j_1k_2} + a^{\dagger}_{k_2}a_{j_1}\delta_{j_2k_1} - a^{\dagger}_{;k_1}a_{j_1}\delta_{j_2k_2} + a^{\dagger}_{k_1}a^{\dagger}_{k_2}a_{j_2}a_{j_1},
\end{aligned} \tag{C3}$$

and thus

$$\begin{aligned}
\left[a^{\dagger}_{k_1}a^{\dagger}_{k_2}, a_{j_2}a_{j_1}\right] &= I_{\mathcal{H}_{\mathcal{F}}}\delta_{j_2k_1}\delta_{j_1k_2} - I_{\mathcal{H}_{\mathcal{F}}}\delta_{j_2k_2}\delta_{j_1k_1} + a^{\dagger}_{k_2}a_{j_2}\delta_{j_1k_1} - a^{\dagger}_{k_1}a_{j_2}\delta_{j_1k_2}\\
&\quad - a^{\dagger}_{k_2}a_{j_1}\delta_{j_2k_1} + a^{\dagger}_{k_1}a_{j_1}\delta_{j_2k_2}.
\end{aligned} \tag{C4}$$

## Second quantization map

By considering the restrictions of $a^{\dagger}_{j}$ to $\mathcal{H}^N$, i.e. $a^{\dagger}_{j}P_{\mathcal{H}^N}$, for $0 \le N \le \infty$ one obtains

$$\begin{aligned}
a^{\dagger}_{j} &= \left|\varphi_j\right\rangle\langle\phi| + \sum_{1\le N\le\infty}\ \sum_{1\le j_1<\cdots<j_N\le\infty}\left|\varphi_j\varphi_{j_1}\ldots\varphi_{j_N}\right\rangle\left\langle\varphi_{j_1}\ldots\varphi_{j_N}\right|\\
&= \sum_{0\le N\le\infty}\ \sum_{1\le j_1<\cdots<j_N\le\infty}\left|\varphi_j\varphi_{j_1}\ldots\varphi_{j_N}\right\rangle\left\langle\varphi_{j_1}\ldots\varphi_{j_N}\right|
\end{aligned}$$

$$= \left|\varphi_j\right\rangle \langle\phi| \wedge \sum_{0\le N\le\infty} \sum_{1\le j_1<\cdots<j_N\le\infty} \left|\varphi_{j_1}\ldots\varphi_{j_N}\right\rangle\left\langle\varphi_{j_1}\ldots\varphi_{j_N}\right|$$
$$= \left|\varphi_j\right\rangle \langle\phi| \wedge \sum_{0\le N\le\infty} P_{\mathcal{H}^N} = \left|\varphi_j\right\rangle \langle\phi| \wedge I_{\mathcal{H}_\mathcal{F}}. \tag{D1}$$

thus one can define the second quantization map $\Gamma$

$$\Gamma : \mathcal{F} \to \mathcal{F} \tag{D2}$$

from the Fock algebra to itself by

$$\Gamma\left(\left|\varphi_j\right\rangle\langle\phi|\right) = a_j^\dagger = \left|\varphi_j\right\rangle \langle\phi| \wedge I_{\mathcal{H}_\mathcal{F}}. \tag{D3}$$

Thus annihilators can be expressed in an analogous fashion by

$$a_j = |\phi\rangle\left\langle\varphi_j\right| + \sum_{1\le N\le\infty} \sum_{1\le j_1<\cdots<j_N\le\infty} \left|\varphi_{j_1}\ldots\varphi_{j_N}\right\rangle\left\langle\varphi_j\varphi_{j_1}\ldots\varphi_{j_N}\right|$$
$$= \sum_{0\le N\le\infty} \sum_{1\le j_1<\cdots<j_N\le\infty} \left|\varphi_{j_1}\ldots\varphi_{j_N}\right\rangle\left\langle\varphi_j\varphi_{j_1}\ldots\varphi_{j_N}\right|. \tag{D4}$$

and

$$a_j = \Gamma\left(|\phi\rangle\left\langle\varphi_j\right|\right) = |\phi\rangle\left\langle\varphi_j\right| \wedge I_{\mathcal{H}_\mathcal{F}}.$$

In a similar fashion

$$a_{l_1}^\dagger a_{m_1} = \Gamma\left(\left|\varphi_{l_1}\right\rangle\left\langle\varphi_{m_1}\right|\right)$$
$$= \sum_{\substack{0\le N,M\le\infty \\ 1\le j_1<\cdots<j_N\le\infty \\ 1\le k_1<\cdots<k_M\le\infty}} \left|\varphi_{l_1}\varphi_{j_1}\ldots\varphi_{j_N}\right\rangle\left\langle\varphi_{j_1}\ldots\varphi_{j_N}\right|\left.\varphi_{k_1}\ldots\varphi_{k_M}\right\rangle\left\langle\varphi_{m_1}\varphi_{k_1}\ldots\varphi_{k_M}\right|$$
$$= \sum_{1\le N\le\infty} \sum_{1\le j_1<\cdots<j_N\le\infty} \left|\varphi_{l_1}\varphi_{j_1}\ldots\varphi_{j_N}\right\rangle\left\langle\varphi_{m_1}\varphi_{j_1}\ldots\varphi_{j_N}\right| = \left|\varphi_{l_1}\right\rangle\left\langle\varphi_{m_1}\right| \wedge I_{\mathcal{H}_\mathcal{F}}. \tag{D5}$$

and

$$a_{l_1}^\dagger a_{l_2}^\dagger a_{m_2} a_{m_1} = \Gamma\left(\left|\varphi_{l_1}\varphi_{l_2}\right\rangle\left\langle\varphi_{m_1}\varphi_{m_2}\right|\right)$$
$$= \sum_{\substack{0\le N,M\le\infty \\ 1\le j_1<\cdots<j_N\le\infty \\ 1\le k_1<\cdots<k_M\le\infty}} \left|\varphi_{l_1}\varphi_{l_2}\varphi_{j_1}\ldots\varphi_{j_N}\right\rangle\left\langle\varphi_{j_1}\ldots\varphi_{j_N}\right|\left.\varphi_{k_1}\ldots\varphi_{k_M}\right\rangle\left\langle\varphi_{m_1}\varphi_{m_2}\varphi_{k_1}\ldots\varphi_{k_M}\right|$$
$$= \sum_{1\le N\le\infty} \sum_{1\le j_1<\cdots<j_N\le\infty} \left|\varphi_{l_1}\varphi_{l_2}\varphi_{j_1}\ldots\varphi_{j_N}\right\rangle\left\langle\varphi_{m_1}\varphi_{m_2}\varphi_{j_1}\ldots\varphi_{j_N}\right|$$
$$= \left|\varphi_{l_1}\varphi_{l_2}\right\rangle\left\langle\varphi_{m_1}\varphi_{m_2}\right| \wedge I_{\mathcal{H}_\mathcal{F}}. \tag{D6}$$

One *should note* that in general

$$\Gamma(A)\,\Gamma(B) \neq \Gamma(A \wedge B) \neq \Gamma(AB), \tag{D7}$$

so $\Gamma$ is not an algebraic map.

### States of a fixed number of electrons

**Theorem 4** *A state $f$ is a $N$ electron state iff $f(\mathcal{N}_1) = N$ and $f(\mathcal{N}_2) = \binom{N}{2}$ i.e. $f(\mathcal{N}_1) = N$ and $f(\mathcal{N}_2) = \binom{N}{2} \Leftrightarrow f\left((\mathcal{N}_1)^2\right) = f(\mathcal{N}_1)^2 = N^2$*

*Proof* In the following we use the operator identity $\left(\mathcal{N}_1\right)^2 = \mathcal{N}_1 + 2\mathcal{N}_2$.
If

$$f(\mathcal{N}_1) = N \text{ and } f(\mathcal{N}_2) = \binom{N}{2} \tag{E1}$$

then

$$f(\mathcal{N}_1 + 2\mathcal{N}_2) = f\left(\mathcal{N}_1^2\right) = N + \frac{2N(N-1)}{2} = N^2 = f(\mathcal{N}_1)^2 \tag{E2}$$

thus $f$ is a pure $N$-electron state. The only if part is trivial as $f(\mathcal{N}_1)^2 = N^2$ clearly implies that $f(\mathcal{N}_1) = N$ and $f(\mathcal{N}_2) = \binom{N}{2}$. □

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