QUANTUM INFORMATION APPROACH TO CORRELATIONS IN MANY-BODY SYSTEMS

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ABSTRACT

QUANTUM INFORMATION APPROACH TO CORRELATIONS IN MANY-BODY SYSTEMS

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Quantum correlations are crucial features in both quantum information theory and many-body physics. Characterization and quantification of quantum correlations have delivered a rich body of work and helped to understand some quantum phenomena. Entanglement is a unique quantum correlation for which it is a resource in many quantum information tasks. Developed for quantification of entanglement, entanglement witness formalism is a remarkable tool in the quantum information toolkit. It can be deployed beyond the entanglement theory to quantify quantum correlations in many-body systems. For many-body systems, the particle statistics and indistinguishability are essential. The relation between indistinguishability and entanglement has to be studied carefully. In this thesis, first, a class of witness operators for pairing correlations in both fermionic and bosonic systems have been proposed and the necessary and sufficient conditions for being a witness operator are found. Then, a Clauser-Horne-Shimony-Holt type test and its bounds for fermions have been demonstrated.

Keywords: Entanglement, identical particles, quantum information, quantum corre-

lations, pairing

ÖZ

ÇOK PARÇALI SİSTEMLERDE KORELASYONLARA KUANTUM BİLİŞİMİ YAKLAŞIMI

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Kuantum korelasyonlarının hem kuantum bilişim kuramında hem de çok parçalı sistemlerde önemli bir yeri vardır. Kuantum korelasyonlarının nitelikleri ve nicelikleri çok geniş bir araştırma konusu olduğu gibi bazı kuantum olgularının anlaşılmasında da yardımcı olmuştur. Dolanıklık, bir çok kuantum bilişim işleminin gerçekleşmesini sağlayan özel bir kuantum korelasyonudur. Dolanıklık tanık formalizmi kuantum bilişim kuramı içerisinde, dolanıklık ölçülmesi için ortaya koyulmuş güçlü bir yöntemdir. Bu yöntem dolanıklık kuramının ötesinde, çok parçalı sistemlerde korelasyonların ölçülmesi için de kullanılabilir. Çok parçalı sistemlerde, parçacık istatistiği ve ayırt edilemezliği ayrıca çok önemlidir. Ayırt edilemezlik ile dolanıklık ilişkisinin dikkatle ele alınması gerekir. Bu tezde, önce fermiyonik ve bozonik sistemler için bir grup çiftleşim korelasyonları tanığı işlemcisi önerilmiş ve tanık işlemcisi olabilmeleri için yeterli ve gerekli koşullar gösterilmiştir. Sonra, fermiyonlar için bir Clauser-Horne-Shimony-Holt türü test ve bu testin limitleri ortaya koyulmuştur.

Anahtar Kelimeler: Dolanıklık, özdeş parçacıklar, kuantum bilişim, kuantum korelas-
yonlar, çiftleşim

To my sweet Aylin, her presence was the last missing thing in completion of this work, to her mother Gül the person who makes me believe I am the luckiest person alive and to my parents Eser and Rükneddin, my sister Ceren, and Abdullah and Candan Çorbacıoğlu for their invaluable support, love and patience.

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CHAPTER 1

INTRODUCTION

Since the seminal works of John Stuart Bell [14] which have shown that quantum mechanics must be nonlocal and Clauser, Horne, Shimony and Holt [22] which introduced a test to nonlocality, entanglement has been the central subject of a great body of work in physics. Arthur Ekert's quantum cryptography and Peter Shor's factorization algorithm [19] had made the interest in the subject grow extraordinarily. The promise that quantum computers can beat the classical computation limits has not only attracted physicists but also government agencies and technology companies around the world [66]. Quantum computers do not only promise faster computations but also render impossible tasks in classical computers into somewhat everyday tasks. Regardless of this kind of power, entanglement is still an elusive property of quantum mechanics and lies at the heart of debates revolving around the nature of reality.

Entanglement is a unique kind of quantum correlation usually defined for spatially distinct parties. This notion seems natural in quantum information theory because of the fact that quantum information tasks are especially designed for spatially separated or distinguishable parties which utilize entanglement for the execution of quantum information tasks. In order to achieve their goal, the entanglement sharing parties may need to perform some operations, for instance measurements, in their laboratories. Obviously, these operations are done locally and the parties may need to classically communicate to coordinate and decide on the local operations they should do on in their laboratories. This general setting is known as *local operations and classical communications (LOCC)*.

Quantum correlations is a rich subject beyond entanglement. Another interesting aspect of entanglement is that, despite the fact entangled states were born out of looking nonlocality in quantum mechanics, nonlocality can exist beyond entangled states [16]. Indeed, all entangled states exhibit nonlocality [53]. Nevertheless, it is widely accepted in physics community that alongside with contexuality, entanglement has solidified the validity of quantum mechanics against alternative theories.

From a foundational and information theoretic point of view the importance of entanglement is indisputable. Another growing field in entanglement theory is entanglement in many-body systems. In recent years a plethora of papers were published for both characterizing and quantification of entanglement in various kinds of systems such as spin chains, Bose-Einstein condensates, Mott insulators, Majorana fermions, superconductors, fermionic gases [5]. Since these many-body systems are fundamentally different than space-like separated parties, for obvious reasons, it requires a delicate approach to define entanglement in these systems.

The ground breaking work of Bardeen, Cooper and Schrieffer [9] has shown the importance of pairing. Pairing has strikingly been successful to explain superconductivity and its explanatory power is not limited to it. It is realized that internal (spin) states of paired electrons can be used to generate entangled states [51, 67, 68]. This clearly shows the relation between pairing and entanglement. However, entanglement is useless from a quantum information viewpoint, unless there is access to it.

This work aims to incorporate tools from entanglement theory to correlations in many-body systems. In chapter 2, separability, entanglement measures, witness formalism, and different approaches to the problem of particle indistinguishability and entanglement are reviewed. In chapter 3, quantification of pairing correlations using the witness formalism was presented with the necessary and sufficient conditions. In chapter 4 we introduce a CHSH test for correlations in fermionic Fock space. The work presented in chapter 3 is published in [1].

CHAPTER 2

ENTANGLEMENT, WITNESS FORMALISM AND PARTICLE INDISTINGUISHABILITY

Characterization and quantification of entanglement is central in entanglement theory [41]. Along with non-commutativity, entanglement is one of the facets of quantum theory that non-locality is rooted in [20]. Quantum information and computation science has become a major research area. Testing the ideas and concepts from quantum information on many-body systems has also attracted a lot of interest. One such endeavor is studying entanglement in many-body systems. Some of the pioneering works are measuring entanglement in Bose-Einstein condensates, atoms trapped in optical lattices, area law and entanglement in spin models [5].

Particle identity is a fundamental trait of quantum mechanics. Almost all of the different properties of different many-body systems has its origins on particle statistics. Symmetrized or anti-symmetrized wavefunctions, in other words permutation of particle labels may give the impression of entanglement. Therefore entanglement of indistinguishable particles has to be treated carefully.

In this chapter first separable state definition will be introduced as convex combination of product states. Then, some fundamental entanglement measures and the entanglement witness formalism will be presented. Finally, there is a review of different approaches on particle indistinguishability and entanglement.

2.1 Entanglement

Quantum states are represented on their own Hilbert spaces. Suppose that quantum systems A and B and their corresponding Hilbert spaces are $\mathcal{H}_A$ and $\mathcal{H}_B$. Then, the Hilbert space of the composite system AB is $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$. If the states of subsytems comprising the total quantum system are exactly known, their state representations are said to be *pure*. The pure product states on $\mathcal{H}_{AB}$ are of the form $|\psi\rangle_{AB} = |\phi\rangle_A \otimes |\phi\rangle_B$ or in short $|\psi\rangle_{AB} = |\phi_A \phi_B\rangle$. However, usually states of subsystems are not pure but a probabilistic mixture of pure states $\rho_A^i = |\phi_A^i\rangle \langle\phi_A^i|$, then $\rho_A = \sum_i p_i \rho_A^i$; where $\sum_i p_i = 1$. The separable mixed states of a bipartite system are convex combinations of bipartite product states $\rho_A \otimes \rho_B$;

$$\rho_{sep} = \sum_{\mu} \lambda_\mu \rho_A^\mu \otimes \rho_B^\mu \tag{2.1}$$

where $\sum_\mu \lambda_\mu = 1$. Pure product states $\rho_A^i \otimes \rho_B^j = |\phi_A^i\rangle \langle\phi_A^i| \otimes \left|\phi_B^j\right\rangle \left\langle\phi_B^j\right|$ where $\text{Span}\left\{\left|\phi_{A(B)}^{i(j)}\right\rangle\right\} = \mathcal{H}_{A(B)}$ are the extremal points of this subset. Every member of this subset can be represented as a convex combination of its extremal points, namely the pure product states. These mixed separable state are in the form of (2.1). All bipartite separable states are a subset of all states. This has a clear geometrical meaning which is pictured in the figure below. A geometrical treatment of quantum states can be found in [15].

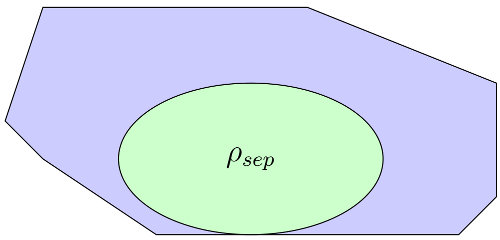


Figure 2.1: The set of all separable states is a subset of all states.

However, this picture is not completely true since the extremals of separable state set is also the extremals of the complete state set.

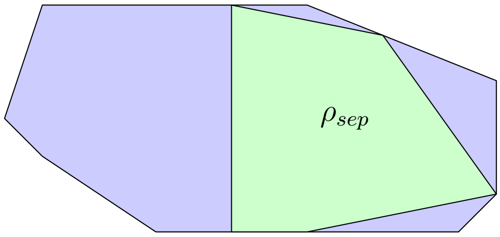


Figure 2.2: A more accurate illustration of separable state set inside the set of all states.

Definition 1. ***Schmidt Decomposition***
There exist ortohormal bases $\{|i_{A(B)}\rangle\}$ *for* $\mathcal{H}_{A(B)}$*, any pure state of the bipartite system* $|\psi_{AB}\rangle = \sum_{m,n} A_{mn} |e_m^A\rangle |e_n^B\rangle$ *with subsystem dimensions* d_A *and* d_B *can be represented in the form of* $|\psi_{AB}\rangle = \sum_i^r c_i |i_A i_B\rangle$ *where* $\sum |c_i|^2 = 1$ *and* $r \leq min(d_A, d_B)$*. This is the Schmidt decomposition of* $|\psi_{AB}\rangle$ *and* c_i *are called Schmidt coefficients.*

This is easily shown by using singular value decomposition of $A = UDV$ where $A_{mn} = U_{mi} D_{ii} V_{in}$, $U_{mi} |e_m^A\rangle = |i_A\rangle$, $V_{in} |e_n^B\rangle = |i_B\rangle$ and $D_{ii} = c_i$.

An immediate observation is that if more than one of the Schmidt coefficients are non-zero then $|\psi_{AB}\rangle$ is an entangled state. The number of non-zero Schmidt coefficients r is called Schmidt rank. So that, ρ is entangled if $r > 1$.

The elementary entanglement quantification is the entropy of entanglement;

$$S_{ent} = -\mathrm{tr}(\rho \log_2 \rho). \tag{2.2}$$

For bipartite pure states this can be calculated by first finding the Schmidt decomposition then using the Schmidt coefficients c_i; $S = \sum_i |c_i|^2 \log_2 |c_i|^2$.

Schmidt decomposition of a pure bipartite state reveals if the state is entangled. However, deciding if any given mixed states is entangled requires a different procedure. If a given bipartite mixed states can be represented as 2.1 it is separable. The elementary entanglement test for bipartite mixed states is the Peres-Horodecki, also known as Positive Partial Transpose (PPT) criterion.

Suppose that X is an operator acting on $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$. A and B act on $\mathcal{H}_A$ and $\mathcal{H}_B$ respectively. Then, we can write down $X = \sum x_{ij,\mu\nu} \left|i\right\rangle \left\langle j\right| \otimes \left|\mu\right\rangle \left\langle \nu\right|$. A partial transpose of X with respect to B is $X^{T_B} = \sum x_{ij,\mu\nu} \left|i\right\rangle \left\langle j\right| \otimes \left|\nu\right\rangle \left\langle \mu\right|$ or $X = \sum x_{ij,\nu\mu} \left|i\right\rangle \left\langle j\right| \otimes \left|\mu\right\rangle \left\langle \nu\right|$. The significance of partial transpose is that if $X = A \otimes B$ that is X is a separable operator then a partial transposition of X with respect to A or B would yield a positive operator otherwise the result is a negative operator. This criteria is necessary and sufficient for dimensions 2×2 and 2×3.

Adopting this result to density operators if $\rho = \sum \rho_{ij,\mu\nu} \left|i\right\rangle \left\langle j\right| \otimes \left|\mu\right\rangle \left\langle \nu\right|$ and partial transpose of ρ with respect to B is $\rho^{T_B} = \sum \rho_{ij,\nu\mu} \left|i\right\rangle \left\langle j\right| \otimes \left|\mu\right\rangle \left\langle \nu\right|$ and with respect to A is $\rho^{T_A} = \sum \rho_{ji,\mu\nu} \left|i\right\rangle \left\langle j\right| \otimes \left|\mu\right\rangle \left\langle \nu\right|$. Then PPT criteria concludes that if $\rho^{T_B} < 0$ or $\rho^{T_A} < 0$ then ρ is an inseparable state. Actually, negativity of one of the partial transposes guarantees negativity of the other.

Despite, its usefulness for $dim = 2 \times 2$ or $dim = 2 \times 3$ systems, PPT criteria fails to be sufficient for higher dimensions [40]. In the literature there are many other entanglement criteria, some being stronger but extremely difficult to compute. Also note that, PPT criteria is an abstract, purely mathematical tool which cannot be applied in laboratory, and requires full knowledge of the state.

2.1.1 Entanglement Measures

Entanglement measurement is one of the pillars of entanglement theory. Some quantum information tasks require manipulation of entangled states and success of these tasks may depend on the amount of entanglement. Also, there is the problem of state transformation. Some states can be converted into another one by *local operations and classical communication* if and only if the final state is not more entangled than the initial state. A comprehensive review for entanglement measures can be found in [65].

An entanglement measure E satisfies the following properties:**1) Monotonicity under *LOCC***: The parties sharing a quantum state can apply *local operations* on the parts they have access and and these parties can talk to each other through *classical communication*, and manipulate the quantum state they share. The final state after this manipulation cannot have more entanglement than the initial state. This *LOCC paradigm* implies an operational context to E. Let Λ be a LOCC protocol then, $E(\Lambda(\rho)) \leq E(\rho)$. **2) Zero for separable states**: An entanglement measure E must be zero for any separable state $E(\rho_{sep}) = 0$. **3) Convexity**: Mixture of entangled states cannot increase total entanglement on average $E(\sum_i p_i \rho_i) \leq \sum_i p_i E(\rho_i)$

- **Concurrence**: $C(\rho) = max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}$ is the concurrence of a mixed qubit state where λ_i's are eigenvalues of the matrix R in decreasing order. The matrix R is defined as $R = \sqrt{\sqrt{\rho}\tilde{\rho}\sqrt{\rho}}$ with $\tilde{\rho} = (\sigma_y \otimes \sigma_y)\,\rho^*\,(\sigma_y \otimes \sigma_y)$ is time reversed form of ρ.

- **Entanglement of Formation**: $E_F = \inf\limits_{p_i, \rho_i} \sum\limits_i p_i E(\rho_i)$ is the convex roof extension of a pure state measure E and infimum is taken over all possible decompositions of ρ. For instance,if E is chosen as the entanglement entropy for a bipartite state of ρ_{AB}, $E_F = \inf\limits_{p_i, |\psi_{AB}\rangle_i} \sum\limits_i p_i S(\rho_{A,i}), \quad \rho_{A,i} = \mathrm{tr}_B(|\psi_{AB}\rangle_i \langle\psi_{AB}|_i)$. However, it is extremely difficult to find an analytical closed form for E_F. For two qubits, E_F can be calculated from concurrence
$$E_F(\rho) = h\left(\frac{1 + \sqrt{1 - C^2(\rho)}}{2}\right)$$
where $h(x) = -x\log_2 x - (1-x)\log_2(1-x)$.

- **Distillable Entanglement**: Most of the important tasks in quantum information and computation deploy maximally entangled states as resources. Therefore, creation of these states is a vital job. Suppose there are a large number, n, of copies of a state ρ. The goal is using an LOCC protocol Λ to transform $\rho^{\otimes n}$ to $\Phi_{2^{rn}} = |\phi_+\rangle\langle\phi_+|^{\otimes rn}$. This kind of LOCC protocols are called *distillation*.
$$E_D(\rho) = \sup\left\{r : \lim_{n\to\infty}\left[\inf_\Lambda \|\Lambda\left(\rho^{\otimes n}\right) - \Phi_{2^{rn}}\|_1\right] = 0\right\}$$
where $\|\cdot\|_1$ is the trace norm of a matrix M; $\|M\|_1 = \mathrm{tr}(\sqrt{MM^\dagger})$.

- **Entanglement Cost**: Entanglement Cost E_C might be thought as the reverse of E_D. In this case from a large number of singlets, a state ρ will be approximated. E_D measures the number of singlets committed for this purpose.
$$E_C(\rho) = \inf\left\{r : \lim_{n\to\infty}\left[\inf_\Lambda \|\rho^{\otimes n} - \Lambda\left(\Phi_{2^{rn}}\right)\|_1\right] = 0\right\}$$

- **Relative Entropy**: Relative entropy E_R measures the distance of a state ρ from the separable set

$$E_R = \inf_{\sigma} S\left(\rho \| \sigma\right)$$

where the infimum is taken over the separable state set and $S\left(\rho\|\sigma\right) = \operatorname{tr}\left\{\rho \log_2 \rho - \rho \log_2 \sigma\right\}$. Relative entropy measures quantum correlations of a state by comparing to a separable state which does not posses quantum correlations.

- **Logarithmic Negativity**: Based on the virtue of PPT criteria, negativity is the sum of negative eigenvalues in ρ^{T_B}

$$\mathcal{N}(\rho) = \frac{\|\rho^{T_B}\|_1 - 1}{2}.$$

Logarithmic Negativity is defined as, $E_N = \log_2(\|\rho^{T_B}\|_1)$

2.2 Quantum Operations, Completely Positive Maps and Entanglement Witnesses

Quantum operations are convex linear mappings that take a density matrix ρ in $\mathcal{H}$ to ρ' in $\mathcal{H}'$. Let $\mathcal{L}(\mathcal{H})$ be the set of square linear operators on $\mathcal{H}$

$$\begin{aligned} \varepsilon(\rho) &= \rho' \\ \varepsilon\left(\sum_k p_k \rho_k\right) &= \sum_k p_k \varepsilon(\rho_k) \\ \varepsilon : \mathcal{L}(\mathcal{H}) &\longrightarrow \mathcal{L}(\mathcal{H}')\ . \end{aligned} \tag{2.3}$$

ε is trace preserving and positive, $\operatorname{tr}\left(\varepsilon(\rho)\right) = 1$ and $\varepsilon(\rho) \geq 0$. We also require that quantum operations can be applicable on composite systems. Suppose that A is an ancilla added to system X and their joint density matrix is ρ_{AX}. If ε is a quantum operation acting on X and leaving the ancilla A unchanged in ρ_{AX}, then the extension $\varepsilon' = \mathbb{I}_A \otimes \varepsilon$ represents the total operation on ρ_{AX}. So, $\varepsilon'\left(\rho_{AX}\right) = \rho'_{AX}$ and $\varepsilon' : \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_X) \rightarrow \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}'_X)$. Since we require ε' to be a physically realizable operation on ρ_{AX}, we demand the same properties; ε' must be positive and trace preserving.

Definition 2. ***Completely Positive Maps***
If $\varepsilon' = \mathbb{I}_A \otimes \varepsilon$ is positive for any $\mathcal{H}_A$ then ε is a completely positive map. If ε' is a completely positive map, then there exist operators $\{M_i\}$ such that; $\varepsilon'(\rho) = \sum_i M_i \rho M_i^\dagger$. M_i are Kraus Operators and $\sum_i M_i M_i^\dagger = 1$.

Transposition operation which is a positive map, i.e. $T : \mathcal{L}(\mathcal{H}) \to \mathcal{L}(\mathcal{H})$ and it can be redefined to act on one part of a composite Hilbert space. Let T_X be the transposition operation on space $\mathcal{H}_X$. If the composite Hilbert space is $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_X$, then $[\mathbb{I}_A \otimes T_X]$ is the transposition operation on $\mathcal{H}_X$. We already know that partial transposition of entangled states are not positive, they have negative eigenvalues. Therefore transposition is a positive(P) but not a completely positive(CP) map. The fact that there exist maps T such that for a composite state ρ, $[\mathbb{I} \otimes T]\,\rho \ngeq 0$ is the essence of Peres-Horodecki criteria [40].

Definition 3. ***Entangled State***
Suppose T is any positive but not completely positive map. If,

$$[\mathbb{I} \otimes T]\,(\rho) \ngeq 0 \tag{2.4}$$

then ρ is entangled.

2.2.1 Entanglement Witnesses

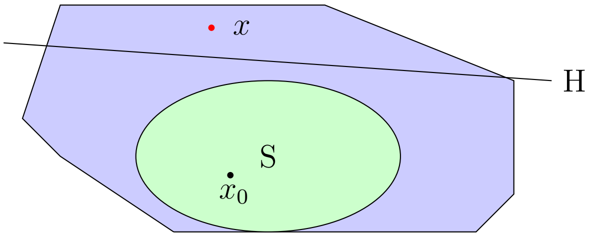
Let D_{AB} be the set of all states and S_{AB} is the subset of all separable states; so that, $\mathrm{S}_{AB} \subset \mathrm{D}_{AB}$. S_{AB} is a convex subset with elements Eq.2.1. The sketch of its geometric interpretation is shown in Fig.s 2.1 and 2.2.

Hyperplane Separation (Hahn-Banach) Theorems

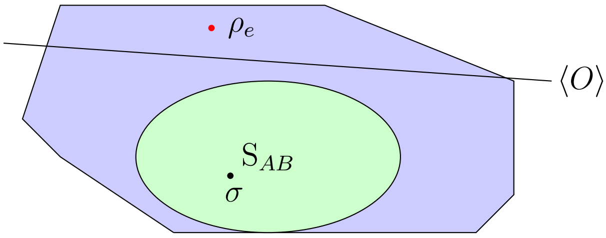
Theorem 1. *If S is a convex set in $\mathbb{R}^n$ and $x \in \mathbb{R}^n$ is a point such that $x \notin \mathrm{S}$, then there exists a hyperplane H that separates S and x such that $dim(\mathrm{H}) = n - 1$ and $\mathrm{H} \cap \mathrm{S} = \varnothing$.*

Corollary 1. *Let S_1 and S_2 be two convex sets in $\mathbb{R}^n$ such that $\mathrm{S}_1 \cap \mathrm{S}_2 = \varnothing$, then there exists a hyperplane that separates S_1 and S_2.*

Note that a single element set is also a convex set. Suppose that ρ_e is an entangled state therefore $\rho_e \notin \mathrm{S}_{AB}$.



(a) Hyperplane H separates x from S



(b) $\langle O \rangle$ defines a hyperplane in D_{AB}

Figure 2.3: Hyperplane separation of a convex subspace

Theorem 2. *Let* S *be a convex linear set,* $x_0 \in \mathrm{S}$ *and* $x \notin \mathrm{S}$*. There is a real linear functional* f *such that;* $\mathsf{f}(x) < c \leq \mathsf{f}(x_0)$.

Suppose $u \in \mathbb{R}^n$ and $c \in \mathsf{R}$, then the set $\mathrm{H} = \{u|\mathsf{f}(u) = c\}$ is a hyperplane in $\mathbb{R}^n$. It is possible to adopt this fact to our needs as follows: Suppose $\rho \in \mathrm{D}_{AB}$ and O is a Hermitian operator, then $\langle \mathrm{O} \rangle = \mathrm{tr}\,(\mathrm{O}\rho) = c$ defines a hyperplane.

$$\begin{aligned} \mathrm{tr}\,(\sigma\mathrm{O}) &\geq c, \forall\, \sigma \in \mathrm{S}_{AB} \\ \mathrm{tr}\,(\rho_e\mathrm{O}) &< c \end{aligned} \tag{2.5}$$

Any operator that obeys above conditions can be minimized over the set of separable states S_{AB}. Let, $m_{sep} = \underset{\rho\,\in \mathrm{S}_{AB}}{min}\, \mathrm{tr}\,(\rho\mathrm{O})$ and define $\tilde{\mathrm{O}} = \mathrm{O} - m_{sep}\mathbb{1}$.

Entanglement Witness [73]
A Hermitian operator W is an entanglement witness if;

$$\begin{aligned} \mathrm{tr}\,(\sigma\mathrm{W}) &\geq 0 \quad \forall\, \sigma \in \mathrm{S}_{AB} \\ \mathrm{tr}\,(\rho_e\mathrm{W}) &< 0 \quad \exists\, \rho_e\,\text{entangled}\,. \end{aligned} \tag{2.6}$$

Witness operators are powerful tools for detecting entanglement in quantum states. They do not require full knowledge of the state and they are experimentally realizable. These are substantially helpful properties for detecting entanglement shared between many particles. It was already discussed that there are maps which are positive when applied to a system but are not necessarily positive when applied on subsystems. These positive but not completely positive maps can detect entanglement. One such map is transposition. Now it will be shown that these maps can be represented as operators which can serve as entanglement witnesses.

Theorem 3. ***Choi-Jamiołkowski Isomorphism*** *Let $\mathcal{A}_1$ and $\mathcal{A}_2$ be linear operator algebras on Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ respectively. $\mathcal{L}(\mathcal{A}_1, \mathcal{A}_2)$ is the space of linear maps from $\mathcal{A}_1$ to $\mathcal{A}_2$. Then there exists a linear transformation $\mathcal{T}$ such that*

$$\mathcal{T} : \Phi \in \mathcal{L}(\mathcal{A}_1, \mathcal{A}_2) \to \mathcal{A}_1 \otimes \mathcal{A}_2,$$

$\mathcal{T}(\Phi)$ is defined through $[\mathcal{T}(\Phi), A_1^\dagger \otimes A_2]_{HS} = [\Phi(A_1), A_2]_{HS}$. $[.\,,.]_{HS}$ is the Hilbert-Schmidt inner product for operator Hilbert spaces and $[A, B]_{HS} = \mathrm{tr}(B^\dagger A)$. The operator form of Φ, denoted as $C_\Phi = \mathcal{T}(\Phi) \in \mathcal{A}_1 \otimes \mathcal{A}_2$, is called Choi operator and can be found by;

$$\mathcal{T}(\Phi) = C_\Phi = (\Phi \otimes \mathbb{1}_{\mathcal{H}_2}) \left(\left|\psi^+\right\rangle \left\langle\psi^+\right| \right) ,$$

where $|\psi^+\rangle = \sum_{i=1}^{d} |e_i\rangle |e_i\rangle$, $d = dim\mathcal{H}_1$ and $\{|e_k\rangle\}$ is an orthonormal basis of $\mathcal{H}_1$.

The Choi-Jamiołkowski isomorphism lets constructing witness operators associated with positive but not completely positive maps

Let $\Lambda : \mathcal{L}(\mathcal{H}_X) \to \mathcal{L}(\mathcal{H}_X)$ be a linear map and let A be an ancilla system with the same dimension; $dim\mathcal{H}_A = dim\mathcal{H}_X = N$. Then, $|\psi^+\rangle_{AX} = \sum_{i=1}^{N} |i\rangle_A \otimes |i\rangle_X$ and $|\psi^+\rangle \langle\psi^+| = \sum_{i,j} |ii\rangle \langle jj| = \sum |i\rangle \langle j|_A \otimes |i\rangle \langle j|_X$. The Choi operator is, then,

$$\begin{aligned} C_\Lambda &= (\mathbb{1}_A \otimes \Lambda_X) (|\Phi\rangle \langle\Phi|) \\ &= \sum_{i,j} |i\rangle \langle j|_A \otimes \Lambda_X (|i\rangle \langle j|_X) \; . \end{aligned} \tag{2.7}$$

This is how Choi operator for a given map is constructed. However, the reverse is also possible and is given as follows:

$$\Lambda(\rho) = \mathrm{tr}_A \left[\left(\mathbb{1}_A \otimes \rho_X^T \right) C_\Lambda \right]$$

The relation between a linear map Λ and its Choi operator C_Λ is crucial if the Choi operator is required to be eligible for being an entanglement witness. Following lemma resolves the question of whether a Choi operator can be an entanglement witness.

Lemma 1. ***a)*** *C_Λ is positive semi-definite if and only if Λ is completely positive*

b) *C_Λ is an entanglement witness if and only if Λ is positive but not completely positive.*

This lemma implies that for any witness operator there is a corresponding positive but not completely positive map. However, finding out this map can be extremely difficult.

2.3 Entanglement and Particle Indistinguishability

In standard quantum information settings, entanglement relies on the fact that entangled parties are distinct entities, whether they are particles or agents (Alice and Bob) that can manipulate the state of the particles they hold, of course this gives the liberty of labeling the particles with the same spatial modes with the agents they belong to. This is the case in the Bell's seminal work or almost all of the quantum information tasks for example teleportation or quantum key distribution [57]. This *"distinctness"* is reflected on the quantification of entanglement as well. However, beyond the usefulness in quantum information tasks, entanglement is a naturally occurring phenomena in systems of many particles where this coincidence between particle labels and spatial modes may not exist. When identical particles colocated, indistinguishability and the definition of entanglement has to be treated carefully.

A simple illustration how particle indistinguishability plays into entanglement is as following: Consider two adjacent wells, separated by a potential large enough to suppress the tunneling. Label the sites L(eft) and R(ight). Suppose each site is occupied by a spin-$\frac{1}{2}$ particle, site L with spin-up and R by spin-down; then the wavefunction of this system is

$$|\Psi\rangle_{dist.} = |\psi_L\rangle \left|\uparrow\right\rangle_L \otimes |\psi_R\rangle \left|\downarrow\right\rangle_R \ . \tag{2.8}$$

The spatial parts of wavefunctions $\psi_{L(R)}(\vec{r})$, have zero overlap. This suggests that for all practical reasons two particles are distinguishable. This permits us to define the composite Hilbert space as the direct product of L and R; $\mathcal{H}_L \otimes \mathcal{H}_R$. Now, at a later time, the potential barrier is lowered and the particles are not localized on sites L and R anymore, and spatial parts of their wavefunctions have nonzero overlap. In this case, since particles are identical, cannot be treated distinguishable. Indices L and R cannot be used to label particles, instead we will enumerate the particles. However note that this enumeration is artificial unlike the site labeling. Using fermion statistics, the new total wavefunction of the system has to be antisymmetrical under particle exchange,

$$|\Psi\rangle_{indist.} = |\psi_L\rangle_1 |\uparrow\rangle_1 |\psi_R\rangle_2 |\downarrow\rangle_2 - |\psi_L\rangle_2 |\uparrow\rangle_2 |\psi_R\rangle_1 |\downarrow\rangle_1 \ . \tag{2.9}$$

This can be seen by $1 \leftrightarrow 2$ leads to

$$\mathrm{P}_{12} |\Psi\rangle_{indist.} = - |\Psi\rangle_{indist.} \ .$$

Now the Hilbert space of the system is not direct product but the anti-symmetric subspace $\mathcal{A}\left(\mathcal{H}_L \otimes \mathcal{H}_R\right)$. The distinguishable state 2.8 is not entangled does not have any quantum correlation, however the indistinguishable state 2.9 has the impression of an entangled state.

Quantum mechanics demand particle exchange symmetry in representing wavefunctions of multiple identical particles. So that, wavefunctions are either symmetric or antisymmetric under particle exchange for Fermionic and Bosonic statistics respectively. If we apply particle exchange symmetry to two identical particles;

$$\begin{aligned}
\mathcal{A}\left(|\psi_L\rangle_1 |\psi_R\rangle_2\right) &= \frac{1}{\sqrt{2}}\left(|\psi_L\rangle_1 |\psi_R\rangle_2 - |\psi_L\rangle_2 |\psi_R\rangle_1\right) \\
\mathcal{S}\left(|\psi_L\rangle_1 |\psi_R\rangle_2\right) &= \frac{1}{\sqrt{2}}\left(|\psi_L\rangle_1 |\psi_R\rangle_2 + |\psi_L\rangle_2 |\psi_R\rangle_1\right)
\end{aligned} \tag{2.10}$$

where particles 1 & 2 are permuted. For a general N particle case, let $|\Psi\rangle_N = |\mu_1, \mu_2, \ldots, \mu_N\rangle$ be non-permuted and ordered where $|\mu_l\rangle_j$ is the j-th particle in state $|\mu_l\rangle$. Note that $|\mu_l\rangle$ are single particle states and $|\mu_l\rangle \in \mathcal{H}_L^{(1)}$ where $\mathcal{H}_L^{(1)}$ is the L-dimensional single particle state. Hilbert space of N identical particles is the (anti)symmetric subspace of $\mathcal{H}^{(N)} = \bigotimes^N \mathcal{H}_L^{(1)}$ for (fermions)bosons. In order to define the wavefunctions for N fermions or bosons, all possible particle permutations $\mathrm{P} \in \mathrm{S}_N$ (S_N is the permutation symmetry group of N items) has to be considered

$$\Sigma_{\pm}\left(|\Psi\rangle_N\right) = \frac{1}{\sqrt{N!}} \sum_P (\pm)^{\varepsilon(P)}\, \mathrm{P} \bigotimes^{N} |\mu_l\rangle_j \ , \tag{2.11}$$

$\varepsilon(P)$ is the sign of the permutation and $\Sigma_+ = \mathcal{S}$, $\Sigma_- = \mathcal{A}$.

The states in 2.10 and 2.11 have the appearance of entangled states. However when expressed in second quantized form, this entangled appearance vanishes. Consider the states in 2.10, in occupation number representation this state is $|1\rangle_L |1\rangle_R$, which is indeed a product state. Let $\{a_i^\dagger\}$ be particle creation operators in mode i, then for N-fermions $|n_1, n_2 \ldots n_M\rangle = \prod\limits_i \left(a_i^\dagger\right)^{n_i} |0\rangle$, $n_i = 0, 1$ and for N-bosons $|n_1, n_2, \ldots n_M\rangle = \prod\limits_i \left[\frac{(a_i^\dagger)^{n_i}}{\sqrt{n_i!}} |0\rangle\right]$, where $\sum_i n_i = N$.

There are different approaches to the relation between particle exchange symmetry and entanglement, and it is still an active debate in quantum information community. Here is given a non-exhaustive review of most notable approaches. A great body of work dismisses the legitimacy of entanglement from (anti)symmetrization [28,30,31, 52,62,69,70,82,84], calling it either unphysical or inaccessible.

Schliemann et. al [69] claim that correlations coming solely from (anti)symmetrization should be excluded from entanglement. They propose a new entanglement criteria based on Slater determinants for fermions. They claim that any fermionic state that cannot be written as a single Slater determinant is quantum correlated, an approach analogous to Schmidt decomposition of distinguishable particles. Note that the same authors cautiously distinguish these correlations from entanglement and prefer to refer to them as quantum correlations.

Let f_i be a set of fermionic annihilation operators. Fermionic operators obey canonical anticommutation relations (CAR)

$$\{f_i, f_j^\dagger\} = f_i f_j^\dagger + f_j^\dagger f_i = \delta_{ij}\ , \{f_i^\dagger, f_j^\dagger\} = \{f_i, f_j\} = 0\,.$$

A general two-fermion state is $|\psi_F\rangle = \sum_{i,j=1}^{m} \omega_{ij} f_i^\dagger f_j^\dagger |vac\rangle$, where $|\psi_F\rangle \in \mathcal{A}(\mathcal{H}_m \otimes \mathcal{H}_m)$. ω is a $m \times m$ antisymmetric, $\omega_{ij} = -\omega_{ji}$, square matrix. Using the fact that there exists a unitary transformation $U : f_i^\dagger \to f_i^\dagger = \sum U_{il} f_l^{\prime\dagger}$ that transforms the antisymmetric $\omega \to \omega' = U\omega U^T$ such that

$$\omega' = Z_0 \oplus Z_1 \oplus Z_2 \oplus \ldots \oplus Z_r$$

where $Z_i = \left[\begin{smallmatrix} 0 & z_i \\ -z_i & 0 \end{smallmatrix}\right]$ and $Z_0 = \mathbf{0}_{m-2r\times m-2r}$. r is the Slater rank of $|\psi_F\rangle$. Any fermionic state with $r > 1$ quantum correlated. This is the *Slater rank criteria* for quantum correlations. Its generalization to bosons(for bosons instead of determinants Slater permanents must be worked out) and N number of particles can be found in [28, 62, 70].

Another approach is partitioning of particles into distinguishable modes. This approach appears a natural adaptation of standard entanglement to identical particles. Modes can be chosen to be locally accessible hence there is an agreement with the LOCC paradigm. A single particle in two distinct modes A and B in second quantized representation is $\frac{1}{\sqrt{2}}[a_A^\dagger + a_B^\dagger]\,|0\rangle = \frac{1}{\sqrt{2}}\,[|1_A 0_B\rangle + |0_A 1_B\rangle]$. Although it seems counterintuitive, a single photon state of this kind has shown to be entangled in [48].

Wiseman and Vacarro [79] point out the fact that entangled states in mode occupation number must obey SSR(superselection rules) and quantum information operations with entangled states of superposition of different number of massive and charged particles are forbidden. They propose that the state of an identical particle system should be projected onto fixed particle number subspaces. For a measure E_M of mode entanglement, true entanglement will be given by, $E_P(|\psi_{AB}\rangle) = \sum_n P_n E_M(|\psi_{AB}^n\rangle)$ where $|\psi_{AB}^n\rangle = \mathbf{\Pi_n}\,|\psi_{AB}\rangle$ and they define E_P as the *entanglement of particles*. Since modes can be chosen differently entanglement depends on the choice of modes. Mode entanglement has been studied in various fermionic, bosonic and spin systems [3, 4, 6, 8, 17, 18, 23–27, 32, 35–38, 47, 55, 59, 60, 71, 75, 76, 80–82, 84].

Another noteworthy approach attempts to find a generalized or unified definition of entanglement based on observable induced subalgebras, in this case entanglement is found observable structure not state space [7, 10, 11, 83].

According to a completely different approach in [42, 77], exchange symmetry causes globally entangled states in fermions and either globally entangled or fully separable states in bosons. They show that permutationally invariant states can be arbitrarily partitioned but else there exists no partitioning, the former implies full separability whereas the later implies global entanglement. Some works propose to obtain useful entanglement from particle indistinguishability without creating any at the process [12, 13, 44, 54, 56, 63]. In a similar spirit, the exchange between particle indistinguishability and entanglement was discussed in [21, 58].

CHAPTER 3

PAIRING CORRELATIONS

Pairing is one of the key aspects of many-body physics. In BCS theory [9] pairing of electrons creates a superconducting state. In low energies, a weak interaction between electrons creates pairs of electrons (known as Cooper pairs), above the Fermi sea thus unstabilizing it. These pairs of electrons behave like bosons and condensate until the system stabilizes and finds a new equilibrium. These pairs of electrons have equal momenta and spin in the opposite directions.

In BCS theory creation of electron pairs are represented by the Cooper pair creation operator

$$\Lambda^\dagger = \sum_k g_k c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow}$$

and the BCS ground state is given by

$$\begin{aligned} |\Psi_{BCS}\rangle &= \exp(\Lambda^\dagger) |0\rangle \\ &= \prod_k \left(1 + g_k c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow}\right) |0\rangle \end{aligned}$$

Cooper pairs in superconductivity might be the most noteworthy pairs in physics but particle pairs can be found in other phenomena such as quantum hall systems [74], bosonic atoms in optical lattices [61, 78], BEC-BCS crossover [49] or superfluidity [64]. Also, it is noteworthy that observation of correlations in time-of-flight experiments can reveal important pairing properties of these quantum systems [2,33,34].

Pairing correlations and entanglement are indeed different quantum correlations interfaced by the indistinguishability of particles. However, it is shown that Cooper pairs can be coherently spatially split into different quantum dots and turned into spin entangled pairs, a process known as Cooper Pair Splitting(CPS) [51, 67, 68]. One of the conceptual challenges for entanglement in many-body systems is to differentiate quantum correlations present in many-body systems from entanglement. Entanglement is an essential resource for quantum information tasks [41] however quantum correlations cannot substitute entanglement in QIT, although as it is noted before quantum correlations can be converted into useful entanglement. An interesting difference is that entanglement is relative to partitioning of a large many-body system on the other hand pairing correlations are not. Pairing correlations are strictly between particles therefore they are basis independent. A system composed of large number of particles and subject to various external parameters, can be virtually partitioned into modes infinitely many different ways. Indeed, entanglement between these partitions will depend on the geometry and size of these partitions. Pairing correlations on the other hand cannot be relative and such artificial partitioning is irrelevant. In [46] measurement and detection of pairing correlations based on witness formalism is discussed. We extend this approach to Bosonic pairing. Bosonic pairing compared to Fermionic pairing is elusive. Nonetheless bosonic pairing is an active research topic [43, 72]. The work in this chapter previously published in [1].

A fermionic state of N independent particles in Hartree-Fock approximation regime

$$|\Psi\rangle = c_1^\dagger c_2^\dagger \cdots c_N^\dagger |0\rangle \ . \tag{3.1}$$

Here $c_i^\dagger$ are creation operators for fermions and $|0\rangle$ is the fermionic vacuum. This state is defined as product state in [69], a state with a single elementary Slater determinant. However, as discussed in Chp.2 for some other approaches with different definition of entanglement, this state Eq. (3.1) is entangled. Kraus et. al. [46] have shown that, there are states which are entangled according to Slater rank criteria but does not have any pairing correlations. Also, they have defined mixtures of states. (3.1) as *separable*. Then non-separable states are quantum correlated. In this work we follow the same separability definitions in [46]. First, witness formalism is borrowed and adopted to pairing correlations then bounds for the witness operator for fermions and bosons are found. In the witness formalism a witness operator quantifies the correlation of a state by its average over the state. It turns out only witness operators of 2-particle operators, $\sum A_{ijkl} c_i^\dagger c_j^\dagger c_k^\dagger c_l^\dagger$ are proper witness operators for pairing correlations.

3.1 Pairing Witness

Only 2-particle observables reveal the pairing correlations. In the following building on this a pairing witnesses will be constructed. Note that there can be many different witness operators for this purpose. We define Q operators as follows:

$$Q = \frac{1}{2} \sum_{ij} A_{ij} c_i c_j \ ,$$

A is a square matrix with complex entries and c_i are particle annihilation operators. Following canonical anticommutaion relations (CAR) and canonical commutation relation (CCR), A is antisymmetric or symmetric respectively. Obviously the former case is fermionic whereas the later one is bosonic. There exist unitary transformation U where $c_i \to c'_i = \sum_j (U^{-1})_{ij} c_j$ and $A \to A' = U^T A U$ such that (i) Fermionic case: $A = \text{diagonal}[A_0, A_1 \cdots A_M]$ with $A_0 = 0$ and $A_i = 2 \times 2$ anti-symmetric blocks and (ii) Bosonic case: A is diagonal. Also it is possible to make A matrices real. We will focus on observables of the form $Q^\dagger Q$. Now we shall assume a unitary transformation suiting our needs are found and Q operators are redefined as,

$$Q = A_1 c_1 c_2 + A_2 c_3 c_4 + \cdots + A_r c_{2r-1} c_{2r} \ \text{(fermions)} \ , \tag{3.2}$$

$$Q = \frac{1}{2}(A_1 c_1^2 + A_2 c_2^2 + \cdots + A_r c_r^2) \ \text{(bosons)} \ , \tag{3.3}$$

where $A_1, \ldots, A_r \in \mathsf{R}^+$. r is the *rank* of Q operator. Unfortunately, it is extremely difficult to solve this problem for arbitrary A's. To simplify and solve the problem we chose $A_1 = A_2 = \cdots = A_r = 1$.

We will denote the largest expectation value of $Q^\dagger Q$ over separable states, with rank r operator Q, by $\Lambda^{\text{sep}}_{r,N}$ such that

$$\Lambda^{\text{sep}}_{r,N} = \sup_{\rho_{\text{sep}}} \operatorname{tr} \rho_{\text{sep}} Q^\dagger Q \ , \tag{3.4}$$

The supremum is taken over the set of separable states ρ_{sep}. The supremum can equivalently be taken over the pure product states $|\Psi_{\text{prod}}\rangle$,

$$\Lambda^{\text{sep}}_{r,N} = \sup_{|\Psi_{\text{prod}}\rangle} \langle \Psi_{\text{prod}} | Q^\dagger Q | \Psi_{\text{prod}} \rangle \ . \tag{3.5}$$

Once the supremum $\Lambda^{\text{sep}}_{r,N}$, we can construct the witness observable

$$W = \Lambda^{\text{sep}}_{r,N}\mathbb{1} - Q^\dagger Q \ . \tag{3.6}$$

If the average of W, is negative which is possible if and only if $\langle Q^\dagger Q\rangle > \Lambda^{\text{sep}}_{r,N}$ then the state is correlated. We will show that the maximum eigenvalue of $Q^\dagger Q$, which will be denoted by $\lambda_{r,N}$, can be larger than $\Lambda^{\text{sep}}_{r,N}$ and this is a necessary and sufficient condition for W to be a witness operator for some correlated states.

3.2 Fermionic Pairing Witness

The Q operator for fermions are already defined as

$$Q = \sum_{i=1}^{r} c_{2i-1}c_{2i} = c_1c_2 + c_3c_4 + \cdots + c_{2r-1}c_{2r} \ . \tag{3.7}$$

We shall define a product state $|\Psi\rangle = c^\dagger_{k_1}c^\dagger_{k_2}\cdots c^\dagger_{k_N}|0\rangle$ where $k_j \in I$ and I is index set for i. First we need to find the maximum expectation values for $\langle Q^\dagger Q\rangle$. Since the average of $\langle Q^\dagger Q\rangle$ is equal to the number of occupied orbitals i where both $2i$ and $2i-1$ are occupied, $N \geq 2r$ $\langle Q^\dagger Q\rangle$ is maximized when all of the first $2r$ orbitals are occupied, hence $\langle Q^\dagger Q\rangle = r$. On the other hand, when $N < 2r$ the maximum of $\langle Q^\dagger Q\rangle$ is achieved by occupying the first N states. As a result,

$$\Lambda^{\text{sep}}_{r,N} = \begin{cases} \lfloor \frac{N}{2} \rfloor & \text{for } N < 2r \ , \\ r & \text{for } N \geq 2r \ . \end{cases} \tag{3.8}$$

For the second half, we need to find $\lambda_{r,N}$. To do so, first define

$$J_x = \frac{Q + Q^\dagger}{2} \tag{3.9}$$

$$J_y = i\frac{Q - Q^\dagger}{2} \tag{3.10}$$

$$J_z = \frac{N_Q - r}{2} \tag{3.11}$$

$$N_Q = \sum_{i=1}^{2r} c^\dagger_i c_i \tag{3.12}$$

and note that since $[J_i, J_j] = i\sum_k \epsilon_{ijk}J_k$. It can be seen that an SU(2) algebra is established. The ladder up and ladder down operators are $Q = J_x - iJ_y$ and $Q^\dagger =$

$J_x + iJ_y$ respectively. Now it is easy to see that $Q^\dagger Q = J^2 - J_z^2 + J_z$. Suppose that $Q\left|\psi_0\right\rangle = 0$ and $N_Q\left|\psi_0\right\rangle = \nu\left|\psi_0\right\rangle$ where $\nu \leq r$. Using the famous angular momentum algebra we can show that $\left|\psi\right\rangle = (Q^\dagger)^\mu\left|\psi_0\right\rangle$ where $0 \leq \mu \leq r-\nu$ is is an eigenstate of $Q^\dagger Q$ with eigenvalue $\mu(r-\nu-\mu+1)$. As a result;

$$\lambda_{r,N} = \max_{0\leq\mu\leq r,N/2} \mu(r+1-\mu) \tag{3.13}$$

$$= \begin{cases} \lfloor\frac{N}{2}\rfloor(r+1-\lfloor\frac{N}{2}\rfloor) & \text{for } N < 2\lfloor\frac{r+1}{2}\rfloor\ , \\ \lfloor\frac{r+1}{2}\rfloor\lceil\frac{r+1}{2}\rceil & \text{for } N \geq 2\lfloor\frac{r+1}{2}\rfloor\ . \end{cases} \tag{3.14}$$

We conclude this part with the following observation: An operator W is a pairing witness if and only if $r > 2$ and $N \geq 2$ consequently $\lambda_{r,N} > \Lambda^{\text{sep}}_{r,N}$.

3.3 Bosonic Pairing Witness

Following the same steps in the fermionic case, first product(unpaired) bosonic states will be defined. Then separation conditions will be calculated. Let $\mathcal{H}_\mathcal{M}$ be M-dimensional bosonic single particle space with annihilation operators $c_i : i = \{1, \ldots M\}$. The operators corresponding to an arbitrary single-particle bosonic state $\phi = [\phi_1, \phi_2 \ldots \phi_M]^T$ can be expand as

$$c(\phi) = \sum_{i=1}^{M} \phi_i^* c_i\ . \tag{3.15}$$

Canonical commutation relations between operators of arbitrary single particle states are then

$$[c(\phi), c^\dagger(\chi)] = \langle\phi|\chi\rangle = \sum_{i=1}^{M} \phi_i^* \chi_i \quad \text{and} \quad [c(\phi), c(\chi)] = 0\ . \tag{3.16}$$

Define a general N-particle bosonic product state as

$$\left|\Psi\right\rangle \simeq c^\dagger(\phi_1)c^\dagger(\phi_2)\cdots c^\dagger(\phi_N)\left|0\right\rangle \tag{3.17}$$

up to a normalization constant and where ϕ_j are single particle states. Note that $\phi_1, \phi_2, \ldots \phi_N$ do not have to be orthonormal, they can be identical or non-orthogonal. Now, it is possible to define two types of product states:

1. **Type 1:** ϕ_j are either mutually orthogonal or mutually identical. Then, it is possible to find an orthonormal set of single particle orbitals $\alpha_1, \ldots, \alpha_p$ that the state is
$$|\Psi\rangle = \frac{(c^\dagger(\alpha_1))^{m_1}}{\sqrt{m_1!}} \cdots \frac{(c^\dagger(\alpha_p))^{m_p}}{\sqrt{m_p!}} |0\rangle \tag{3.18}$$
where m_b is the number of bosons occupying orbital α_b and there are $N = \sum_{b=1}^{p} m_b$ bosons.

2. **Type 2:** The single-particle states $\phi_1, \phi_2, \ldots, \phi_N$ are not necessarily identical or orthogonal. ϕ_i and ϕ_j can overlap therefore $\langle\phi_i|\phi_j\rangle$ can be nonzero.

Name the set of all type-1 product states $\mathcal{S}_1$ and the set of all type-2 product states $\mathcal{S}_2$. It is easy to see that $\mathcal{S}_1 \subset \mathcal{S}_2$. The product states $\rho_{sep} \in \mathcal{S}_1$ can be viewed as a special case of generalized product states $\mathcal{S}_2 \setminus \mathcal{S}_1$. It was discussed before that there are different approaches to indistinguishability and entanglement. According to [30, 31] symmetrized products of single-particle *non-orthogonal* bosonic states are entangled and those of *orthogonal* bosonic states are separable.

For bosons the Q operator is
$$Q = \frac{1}{2}\sum_{i=1}^{r} c_i^2 \ , \tag{3.19}$$

where r is the rank of Q operator. Computation of an analytical result for the largest separable expectation value of $\langle Q^\dagger Q\rangle$ for type-2 product states has shown to be extremely difficult for this case only numerical results for $N \leq 12$ will be provided. In order to compute the largest eigenvalue of $Q^\dagger Q$ first, introduce the following commutation relations:

$$[Q, Q^\dagger] = N_Q + \frac{r}{2} \ , \tag{3.20}$$
$$[N_Q, Q^\dagger] = 2Q^\dagger \ , \tag{3.21}$$

where $N_Q = \sum_{i=1}^{r} c_i^\dagger c_i$ is the number operator for the states $1 \leq i \leq r$. Then note that Q, $Q^\dagger$ and $N_Q + r/2$. Following the same steps in the fermionic case the largest eigenvalue for common eigenstates of commuting $Q^\dagger Q$ will be computed. The ladder operators for this case are $Q^\dagger$ and Q. Let $Q\,|\psi_0\rangle = 0$ is the state annihilated by Q_0 and let $\langle N_Q\rangle_{|\psi_0\rangle} = \nu$ and the total number of bosons of $|\psi_0\rangle$ be $\nu + \nu'$, i.e. $\langle N\rangle_{|\psi_0\rangle} = \nu + \nu'$.

Consequently,

$$|\psi_0\rangle = f(c_1^\dagger, c_2^\dagger, \ldots, c_r^\dagger) g(c_{r+1}^\dagger \ldots) |0\rangle \tag{3.22}$$

where f and g are homogeneous polynomials of degree ν and ν' respectively. Since it is required $Q|\psi_0\rangle = 0$, f is also a solution to r-dimensional Laplacian in r-dimensions. Define

$$|\psi\rangle = (Q^\dagger)^\mu |\psi_0\rangle \tag{3.23}$$

a state with N_Q eigenvalue $\nu + 2\mu$ and N eigenvalue $\nu + \nu' + 2\mu$ Using the above commutation relations it is straightforward to show that

$$Q^\dagger Q |\psi\rangle = \mu(\nu + \frac{r}{2} + \mu - 1) |\psi\rangle \ . \tag{3.24}$$

Now choosing $\mu = \lfloor \frac{N}{2} \rfloor$ and $\nu = 0$ will give the maximum eigenvalue

$$\lambda_{r,N} = \begin{cases} \frac{N(N+r-2)}{4} & \text{if } N \text{ is even,} \\ \frac{(N-1)(N+r-1)}{4} & \text{if } N \text{ is odd.} \end{cases} \tag{3.25}$$

In order to complete constructing the witness presented in Eq. 3.6, the separable bounds for two types of product states are required. The computation for type-1 product states are presented in Appendix A. The separability bounds are

$$\Lambda_{r,N}^{\text{sep(type 1)}} = \begin{cases} \frac{N^2}{4} & \text{if } N \text{ is even,} \\ \frac{N^2-1}{4} & \text{if } N \text{ is odd.} \end{cases} \tag{3.26}$$

Note that the type-1 separability bounds Eq. 3.26 do not depend on rank of Q operators. $p = 2$ in 3.18 is the maximizing states for $Q^\dagger Q$ and since $r \geq 2$ the single particle states lie inside the subspace, h_r, spanned by first r basis states, i.e. $\alpha_1, \alpha_2 \in h_r$.

For type-2 product states separability bounds appear to depend on r. In this case the overlap between single particle states $\phi_1, \ldots, \phi_N$ maximizing $\langle Q^\dagger Q \rangle$ is non-zero and there is a dependency on r. However, as long as the single particle states lie inside h_r the value of r will not change the bound;

$$\Lambda_{r,N}^{\text{sep(type 2)}} = \Lambda_{N,N}^{\text{sep(type 2)}} \quad \text{for } r > N \ . \tag{3.27}$$

There is an important distinction between bounds of type-1 and type-2 separable states for the values $2 \leq r \leq N$ for rank of Q. For type-2 states, it appears that

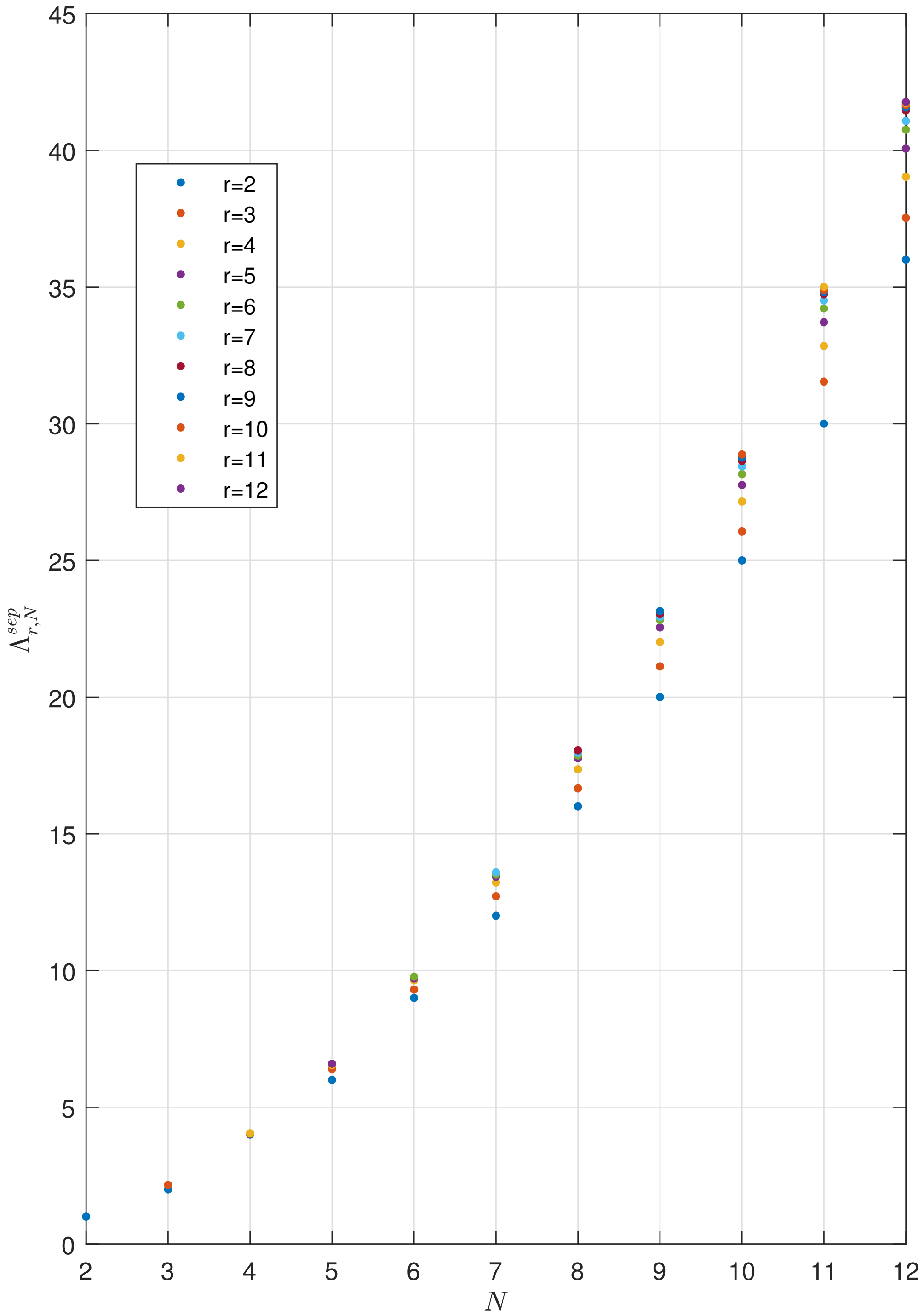


Figure 3.1: Type 2 separable-state bound, i.e., maximum expectation value of $Q^{\dagger}Q$ in type 2 separable states, is plotted as a function of the total number of particles. The bound also depends on the rank r. The lowest markers are for $r = 2$ and the value of r changes by 1 between two successive markers. Note that the value of the bound for $r > N$ is identical with the bound for $r = N$.

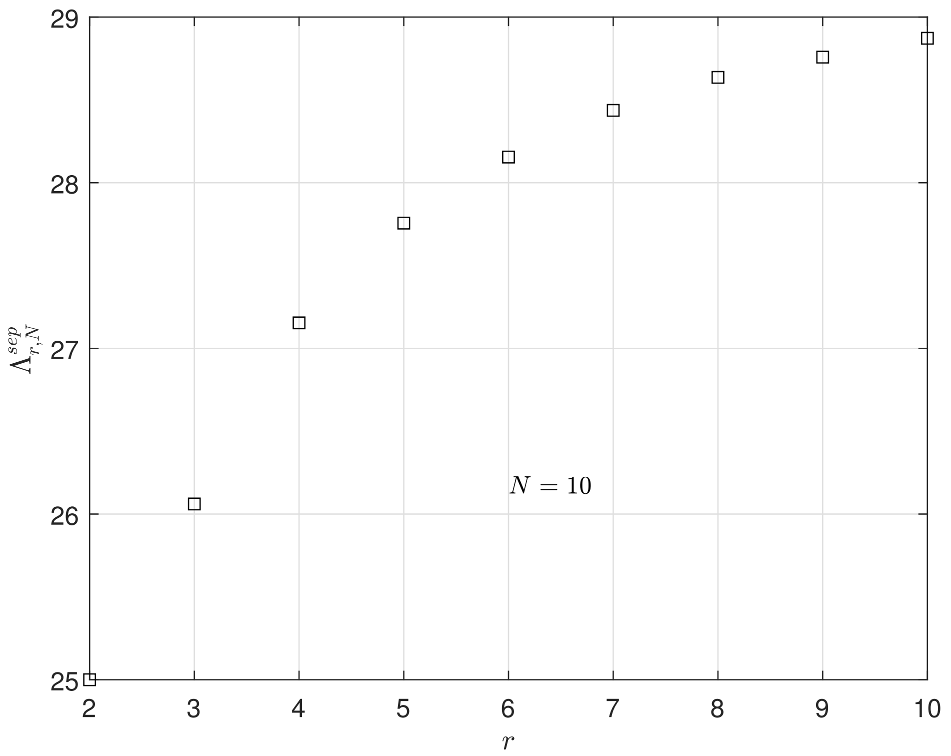


Figure 3.2: Type 2 separable-state bound for $N = 10$ particles for different values of the rank r. The value $r = 2$ is equal to the type 1 bound. Also, note that the bound for $r > N$ is equal to the bound for $r = N$.

the bound increases with r and saturates at $r = N$, this means that a larger measurement range does not increase the accuracy of detection. In fact, experimentally detection is generally very difficult for $Q^\dagger Q$, as can be seen from

$$\frac{\lambda_{r,N}}{\Lambda_{r,N}^{\mathrm{sep(type\,1)}}} \sim \frac{N+r}{N} \,, \tag{3.28}$$

which implies that for large particle systems this violation is extremely small. For the numerically computed parts $N \leq 12$, it appears that separability bounds $\Lambda_{r,N}^{\mathrm{sep(type\,1)}} \sim \Lambda_{r,N}^{\mathrm{sep(type\,2)}}$.

3.3.1 Rank 2 Case

At $r = 2$, $\lambda_{2,N} = \Lambda_{2,N}^{\mathrm{sep(type\,1)}} = \Lambda_{2,N}^{\mathrm{sep(type\,2)}}$. This implies that our choice of witness composed of Q operators does not detect pairing at $r = 2$ since $\lambda_{r,N} > \Lambda_{r,N}^{\mathrm{sep}}$ is the necessary requirement. However, this defect can be fixed for type-1 product states by changing the Q operators in Eq.3.19 to

$$Q'(r=2) = \frac{1}{2}\left(A_1 c_1^2 + A_2 c_2^2\right) \,. \tag{3.29}$$

All the eigenstates of $Q'^\dagger Q'$ are type-2 product states, this is why modifying Q operators at $r = 2$ will not change the situation. Note that $\mathcal{S}_1 \subset \mathcal{S}_2$, i.e. type-1 product states are a subset of type-2 product states there exists rank 2 Q operators that can witness them. This is illustrated in Fig.3.3

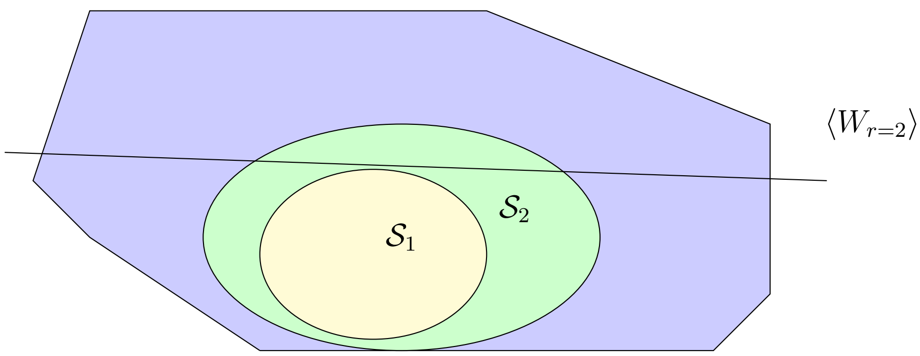


Figure 3.3: $\mathcal{S}_1$ is a subset of $\mathcal{S}_2$, $W_{r=2}$ can witness type-1 product states but not $\mathcal{S}_2 \backslash \mathcal{S}_1$

Table 3.1: The summary of validity of Pairing Witness

	Type 1	**Type 2**
Single particle orbitals are from an orthonormal set	Yes	No
Separability bound depends on the rank of Q	No	for $r < N$ Yes
		for $r \geq N$ No
Witness at rank $r = 2$	No	No

CHAPTER 4

CORRELATION TESTS BY CHSH INEQUALITY

Any Hermitian operator X that has correlated eigenstates can be used as a witness for correlations. In that case, the maximum expectation value in separable states

$$\Lambda_{\text{sep,max}}(X) = \max_{|\psi\rangle \text{ sep}} \langle\psi|X|\psi\rangle \tag{4.1}$$

is expected to be smaller than the maximum eigenvalue $\lambda_{\max}(X)$ of the operator X. Then, for any state, the strict inequality

$$\Lambda_{\text{sep,max}}(X) < \langle X\rangle \tag{4.2}$$

is a proof that the state is separable.

A possible candidate for such an operator is any observable that are used for testing Bell inequalities, which compare locally realistic theories with quantum mechanics, or the contextuality inequalities, which compare non-contextual realistic theories with quantum mechanics. The simplest such observable is

$$X = A_1A_2 + A_2A_3 + \cdots + A_{m-1}A_m - A_mA_1 \ , \tag{4.3}$$

where A_i are dichotomic observables with ± 1 values such that successive observables commute, $[A_i, A_{i+1}] = 0$ ($i = 1, 2, \ldots, m$; we use cyclic order with $A_{m+1} = A_1$). Using realistic theories with either non-contextuality or locality assumption, it is possible to show that

$$\langle X\rangle \leq m - 2 \ . \tag{4.4}$$

However, quantum mechanics violates this bound [29],

$$\lambda_{\max}(X) = m \cos\frac{\pi}{m} \ . \tag{4.5}$$

The case $m = 4$ corresponds to the celebrated Clauser-Horne-Shimony-Holt (CHSH) inequality and the case $m = 5$ corrseponds to the Klyachko-Can-Binicioğlu-Shumovsky (KCBS) inequality [45].

For fermionic systems, the number of fermions in an orbital ($n = c^\dagger c$) is a natural dichotomic variable with two values being 0 and 1. For this reason, the corresponding observable $A = 2n - 1$ is a ± 1 valued dichotomic variable. The main observable X can therefore be expressed either in terms of A operators or the corresponding number operators. Note that the arguments of realism are no longer applicable for many fermion systems. For this reason, there is no reason to expect that the separability bound $\Lambda_{\text{sep,max}}(X)$ obeys the inequality in Eq. (4.4). However, numerical calculations indicate that the separability bound is very close to the realism bound. Unfortunately, there is no known analytical expressions for the bounds. The case $m = 4$, i.e., the analog of CHSH, will be treated below.

4.1 The inequality in terms of the number operators

First, it is necessary to define the mathematical concepts that we will deal with. Let h denote the one-particle Hilbert space for a fermionic many-particle system. In other words, h contains the main orbitals that can be filled with fermions. Suppose that h is d dimensional and let $|1\rangle, |2\rangle, \ldots, |d\rangle$ be an orthonormal basis of h. Let $c_1, c_2, \ldots, c_d$ be the corresponding annihilation operators which satisfy the canonical anti-commutation relations

$$\{c_i, c_j^\dagger\} = \delta_{ij} \ , \tag{4.6}$$

$$\{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0 \ . \tag{4.7}$$

Let $|\alpha\rangle$ be an arbitrary one-particle state in h,

$$|\alpha\rangle = \alpha_1|1\rangle + \alpha_2|2\rangle + \cdots + \alpha_d|d\rangle \ . \tag{4.8}$$

We define the annihilation operator corresponding to the state $|\alpha\rangle$ as

$$c(\alpha) = \alpha_1^* c_1 + \alpha_2^* c_2 + \cdots + \alpha_d^* c_d \ . \tag{4.9}$$

It can be shown easily that the canonical anti-commutation relations can be expressed as follows

$$\{c(\alpha), c^\dagger(\beta)\} = \langle\alpha|\beta\rangle \ , \tag{4.10}$$

$$\{c(\alpha), c(\beta)\} = \{c^\dagger(\alpha), c^\dagger(\beta)\} = 0 \ . \tag{4.11}$$

The number operator for a given one-particle state $|\alpha\rangle$ is defined as

$$n(\alpha) = c^\dagger(\alpha)c(\alpha) \ , \tag{4.12}$$

and has eigenvalues 0 and 1. The commutator of two number operators is

$$[n(\alpha), n(\beta)] = \langle\alpha|\beta\rangle c^\dagger(\alpha)c(\beta) - \langle\beta|\alpha\rangle c^\dagger(\beta)c(\alpha) \ . \tag{4.13}$$

This shows that two different number operators commute if and only if the corresponding single-particle orbitals are orthogonal,

$$(\text{for } \alpha \neq e^{i\vartheta}\beta) \quad [n(\alpha), n(\beta)] = 0 \iff \langle\alpha|\beta\rangle = 0 \ . \tag{4.14}$$

This establishes our compatibility condition.

Now, let's suppose that we have a cyclic list $|\alpha_1\rangle, |\alpha_2\rangle, \ldots, |\alpha_m\rangle$ of m single-particle orbitals (cyclic means $|\alpha_{m+1}\rangle = |\alpha_1\rangle$) such that two succeeding orbitals are orthogonal,

$$\langle\alpha_i|\alpha_{i+1}\rangle = 0 \quad (i = 1, 2, \ldots, n) \ . \tag{4.15}$$

We define $n_i = n(\alpha_i)$ and $A_i = 2n_i - 1$ which will form m dichotomic operators where the successive operators are compatible. Then,

$$X = A_1A_2 + \cdots + A_{m-1}A_m - A_mA_1 \tag{4.16}$$

$$= m - 2 - 4Y \tag{4.17}$$

where

$$Y = (n_2 + \cdots + n_{m-1}) - (n_1n_2 + \cdots + n_{m-1}n_m - n_mn_1) \ . \tag{4.18}$$

The inequality $X \leq m-2$ is equivalent to $Y \geq 0$. However, these are bounds that can be placed by using the appropriate realism argument. For separability, new bounds will be obtained. Let's express these in terms of both a lower and an upper bound,

$$\Lambda_{\text{sep,min}}(X) \leq \langle X\rangle \leq \Lambda_{\text{sep,max}}(X) \ , \tag{4.19}$$

$$\Lambda_{\text{sep,min}}(Y) \leq \langle Y\rangle \leq \Lambda_{\text{sep,max}}(Y) \ . \tag{4.20}$$

where the expectation values are evaluated in separable states. We naturally have $\Lambda_{\text{sep,max}}(X) = m - 2 - 4\Lambda_{\text{sep,min}}(Y)$, etc.

4.2 Bounds for separable states

The separable bound in Eq. (4.1) has to be maximized over all possible separable states formed from all orbitals in h. It will be shown below that, if X is an operator defined by using $c(\alpha_1), \ldots, c(\alpha_m)$ and the corresponding creation operators, then $\Lambda_{\text{sep,max}}(X)$ can be computed by using separable states formed from the orbitals in the linear span of $\alpha_1, \ldots, \alpha_m$.

First, consider an arbitrary separable state with k fermions defined through the creation operators of k orbitals $\beta_1, \ldots, \beta_k$,

$$|\psi\rangle = c^\dagger(\beta_1)c^\dagger(\beta_2)\ldots c^\dagger(\beta_k)|0\rangle \ . \tag{4.21}$$

What is important to notice is that this state actually depends on the linear subspace $\mathcal{V}$ spanned by the k orbitals $\beta_1, \ldots, \beta_k$. In fact, if $\gamma_1, \ldots, \gamma_k$ is another set of orbitals spanning the same subspace, so that there is a $k \times k$ matrix M with

$$\beta_i = \sum_{j=1}^{k} M_{ij}\gamma_k \ , \tag{4.22}$$

then it can be shown that

$$c^\dagger(\beta_1)c^\dagger(\beta_2)\ldots c^\dagger(\beta_k) = (\det M)c^\dagger(\gamma_1)c^\dagger(\gamma_2)\ldots c^\dagger(\gamma_k) \ . \tag{4.23}$$

In other words, the same separable state $|\psi\rangle$ can be defined by filling γ–orbitals as well. The only difference between the two sets of orbitals is the multiplication of $|\psi\rangle$ by a complex number, which doesn't change the corresponding quantum state.

Next, it will be shown that if $|\psi\rangle$ is a separable state (for example, the state in Eq. (4.21)), then

$$|\psi'\rangle = c(\phi_1)\ldots c(\phi_p)|\psi\rangle \tag{4.24}$$

is also a separable state. To show this, consider the subspace $\mathcal{V} = \operatorname{span}\{\beta_1, \ldots, \beta_k\}$ of h. Let $\mathcal{V}^\perp$ be the orthogonal complement of $\mathcal{V}$. Let ϕ_i' and ϕ_i'' be the projection of ϕ_i on the subspaces $\mathcal{V}$ and $\mathcal{V}^\perp$, respectively. Since

$$\phi_i = \phi_i' + \phi_i'' \tag{4.25}$$

and since $c(\phi_i'')|\psi\rangle = 0$, we have

$$|\psi'\rangle = c(\phi_1') \dots c(\phi_p')|\psi\rangle \tag{4.26}$$

At this point, we notice that $\phi_1', \dots, \phi_p'$ spans a p-dimensional subspace of $\mathcal{V}$. Construct a new basis $\omega_1, \dots, \omega_k$ of $\mathcal{V}$ such that the first k vectors span that subspace, i.e.,

$$\mathrm{span}\{\omega_1, \dots, \omega_p\} = \mathrm{span}\{\phi_1', \dots, \phi_p'\} \tag{4.27}$$

$$\mathrm{span}\{\omega_1, \dots, \omega_p, \omega_{p+1}, \dots, \omega_k\} = \mathcal{V} \,. \tag{4.28}$$

Consequently $|\psi\rangle = (\mathrm{const})c^\dagger(\omega_1)\cdots c^\dagger(\omega_k)|0\rangle$ and

$$|\psi'\rangle = (\mathrm{const}')c(\omega_1)\cdots c(\omega_p)|\psi\rangle \tag{4.29}$$

$$= (\mathrm{const}'')c^\dagger(\omega_{p+1})\cdots c^\dagger(\omega_k)|0\rangle \,, \tag{4.30}$$

which is obviously a separable state. We can generalize the above statement as follows: A product of a set of creation and annihilation operators applied to the vacuum state,

$$c(\beta_1)\cdots c(\beta_p)c^\dagger(\gamma_1)\cdots c^\dagger(\gamma_q)c(\delta_1)\cdots c(\delta_r)\cdots c^\dagger(\omega_1)\cdots c^\dagger(\omega_k)|0\rangle \,, \tag{4.31}$$

is a separable state.

Now, to show what we have started with, suppose that X is any operator defined by using creation and annihilation operators of m orbitals $\alpha_1, \dots, \alpha_m$ and let $|\psi\rangle$ be a separable state with M particles. Let $\mathcal{V}$ be a linear span of $\alpha_1, \dots, \alpha_m$. Choose an orthonormal basis $\beta_1, \beta_2, \dots$ of the orthogonal complement $\mathcal{V}^\perp$. The state $|\psi\rangle$ can be expanded in terms of the creation operators of the α and β orbitals. Let

$$|\psi\rangle = \sum_{p=0}^{M} \sum_{k_1<\cdots<k_p} A_{k_1k_2\dots k_p} c^\dagger(\beta_{k_1})c^\dagger(\beta_{k_2})\cdots c^\dagger(\beta_{k_p})|\Phi_{k_1k_2\dots k_p}\rangle \tag{4.32}$$

be that expansion where $A_{k_1k_2\dots k_p}$ are expansion coefficients and each $|\Phi_{k_1k_2\dots k_p}\rangle$ is a normalized state formed from creation operators of α_i, i.e.,

$$|\Phi_{k_1k_2\dots k_p}\rangle = F(c^\dagger(\alpha_1), c^\dagger(\alpha_2), \dots, c^\dagger(\alpha_m))|0\rangle \,, \tag{4.33}$$

for some function F. Now, it can be seen that each $|\Phi_{k_1k_2\dots k_p}\rangle$ is separable because

$$|\Phi_{k_1k_2\dots k_p}\rangle = (\mathrm{Proj})c(\beta_{k_p})\cdots c(\beta_{k_2})c(\beta_{k_1})|\psi\rangle \tag{4.34}$$

where

$$\mathrm{Proj} = c(\beta_1)c^\dagger(\beta_1)c(\beta_2)c^\dagger(\beta_2)\cdots \tag{4.35}$$

is a projection operator on the Fock space that projects to subspaces where all β orbitals are empty.

Computing the expectation value of X in the state in Eq. (4.32), we get

$$\langle X\rangle_\psi = \sum_p \sum_{k_1<k_2<\cdots<k_p} |A_{k_1k_2\ldots k_p}|^2 \langle X\rangle_{\Phi_{k_1\ldots k_p}} . \tag{4.36}$$

This shows that the separable-state expectation value $\langle X\rangle_\psi$ is an average of the separable-state expectation values $\langle X\rangle_{\Phi_{k_1\ldots k_p}}$ where the filled orbitals are from $\mathcal{V}$ subspace. For the case $\langle X\rangle_\psi$ is maximum, all other individual expectation values must be equal to that maximum value. This shows that the maximum value $\Lambda_{\text{sep,max}}(X)$ can be obtained from separable states where all fermions are filled to an orbital in $\mathcal{V}$.

4.3 Computation of $\Lambda_{\text{sep,max}}(X)$

In short, this implies that for the CHSH based expression, which is formed from $m = 4$ orbitals, $\Lambda_{\text{sep,max}}(X)$ can be computed by using 4 orbitals. This is also equivalent to taking the single-particle Hilbert space h to be 4-dimensional. This assumption is made in all of the following analysis.

Let $\Lambda_{\text{sep},max,k}(X)$ be the maximum evaluated from k-particle separable states. By using particle-hole transformation, it is possible to see that

$$\Lambda_{\text{sep},max,k}(X) = \Lambda_{\text{sep},max,4-k}(X) \tag{4.37}$$

For every separable state, $|\psi\rangle = c^\dagger(\gamma_1)\cdots c^\dagger(\gamma_k)|0\rangle$ of k fermions, there is a corresponding state of $4-k$ fermions (equivalently k holes), $|\tilde{\psi}\rangle = c(\gamma_1)\cdots c(\gamma_k)|F\rangle$ where $|F\rangle$ is the state where all 4 orbitals are filled with fermions. This is a transformation that changes each number operator n_i to $1-n_i$. Equivalently, in terms of the $A_i = 2n_i - 1$, the transformation amounts to changing the sign of each A_i. Consequently X is invariant under this transformation. This proves that the maximum separable value of $\langle X\rangle$ for k fermions is equal to the maximum separable value for k holes. The identity above then follows.

For this reason, we need to compute $\Lambda_{\text{sep},min,k}(X)$ and $\Lambda_{\text{sep},max,k}(X)$ for $k = 0, 1, 2$ only. In each case, instead of computing the upper separable bound for X, we are going to check the lower bound $Y \geq 0$ for

$$Y = n_2 + n_3 - (n_1 n_2 + n_2 n_3 + n_3 n_4 - n_4 n_1) \ . \tag{4.38}$$

It is easy to see that

$$\langle 0|Y|0\rangle = 0 \ , \tag{4.39}$$

and therefore

$$\Lambda_{\text{sep},min,0}(Y) = \Lambda_{\text{sep},max,0}(Y) = 0 \ . \tag{4.40}$$

For $k = 1$ fermion states, we have

$$\langle n_i n_{i+1}\rangle = 0 \tag{4.41}$$

because it is not possible that two different orbitals to be occupied at the same time. It is also easy to see that the bounds $0 \leq \langle Y\rangle \leq 1$ is also satisfied for $k = 1$. Consequently,

$$\Lambda_{\text{sep},min,1}(Y) = 0 \ , \tag{4.42}$$

$$\Lambda_{\text{sep},max,1}(Y) = 1 \ . \tag{4.43}$$

What is left is to find the bounds for 2-fermion separable states. First, remember that $\alpha_1, \ldots, \alpha_4$ are a set of orbitals where the successive orbitals are orthogonal to each other. This means that α_1 and α_3 are orthogonal to α_2 and α_4. Let $\mathcal{W}$ be the 2-dimensional subspace spanned by α_1 and α_3. The orthogonal complement $\mathcal{W}^{\perp}$ is therefore spanned by α_2 and α_4.

Consider a 2-fermion separable state

$$|\psi\rangle = c^{\dagger}(\beta_1)c^{\dagger}(\beta_2)|0\rangle \ . \tag{4.44}$$

Let $\mathcal{V}$ be the 2-dimensional space spanned by β_1 and β_2, i.e., the subspace of the occupied orbitals. It is possible to choose the basis $\{\beta_1, \beta_2\}$ for $\mathcal{V}$ such that their projections onto $\mathcal{W}$ are also orthogonal. This also implies the orthogonality of their projections onto $\mathcal{W}^{\perp}$.

At this point, we describe the vectors in h as 4×1 column matrices. Let $\mathcal{W}$ be the space spanned by the first two standard basis vectors. Then, the following assignment of the six vectors is the most general one.

$$\beta_1 = \begin{bmatrix} \cos\frac{\Omega_1}{2} \\ 0 \\ \sin\frac{\Omega_1}{2} \\ 0 \end{bmatrix} \qquad \beta_2 = \begin{bmatrix} 0 \\ \cos\frac{\Omega_2}{2} \\ 0 \\ \sin\frac{\Omega_2}{2} \end{bmatrix} \quad , \tag{4.45}$$

$$\alpha_1 = \begin{bmatrix} \cos\frac{\theta_1}{2} \\ e^{i\varphi_1}\sin\frac{\theta_1}{2} \\ 0 \\ 0 \end{bmatrix} \qquad \alpha_2 = \begin{bmatrix} 0 \\ 0 \\ \cos\frac{\theta_2}{2} \\ e^{i\varphi_2}\sin\frac{\theta_2}{2} \end{bmatrix} \tag{4.46}$$

$$\alpha_3 = \begin{bmatrix} \cos\frac{\theta_3}{2} \\ e^{i\varphi_3}\sin\frac{\theta_3}{2} \\ 0 \\ 0 \end{bmatrix} \qquad \alpha_4 = \begin{bmatrix} 0 \\ 0 \\ \cos\frac{\theta_4}{2} \\ e^{i\varphi_4}\sin\frac{\theta_4}{2} \end{bmatrix} \tag{4.47}$$

The expectation values can be computed as

$$\langle n_i \rangle = |\langle \beta_1|\alpha_i\rangle|^2 + |\langle \beta_2|\alpha_i\rangle|^2 \tag{4.48}$$

$$\langle n_i n_{i+1} \rangle = \left| \det \begin{bmatrix} \langle \beta_1|\alpha_i\rangle & \langle \beta_1|\alpha_{i+1}\rangle \\ \langle \beta_2|\alpha_i\rangle & \langle \beta_2|\alpha_{i+1}\rangle \end{bmatrix} \right|^2 . \tag{4.49}$$

Computing all expressions, we get the following

$$\begin{aligned} \langle Y \rangle = \frac{1}{8}\Bigg(& 6 + 2\cos\Omega_1\cos\Omega_2 + \\ & (1 - \cos\Omega_1\cos\Omega_2)\Big[\cos\theta_1\cos\theta_2 + \cos\theta_2\cos\theta_3 \\ & \qquad + \cos\theta_3\cos\theta_4 - \cos\theta_4\cos\theta_1\Big] \\ & + \sin\Omega_1\sin\Omega_2\Big[\sin\theta_1\sin\theta_2\cos(\varphi_1-\varphi_2) + \sin\theta_2\sin\theta_3\cos(\varphi_2-\varphi_3) \\ & \qquad + \sin\theta_3\sin\theta_4\cos(\varphi_3-\varphi_4) - \sin\theta_4\sin\theta_1\cos(\varphi_4-\varphi_1)\Big]\Bigg) . \end{aligned} \tag{4.50}$$

There are 10 angle variables, each of which appears with a simple trigonometric function in here. We will first find the extrema of this expression with respect to the Ω_i angles.

Extremization with respect to Ω_i appears to be simple as the expression above is of the form

$$\langle Y \rangle = a \cos\Omega_1 \cos\Omega_2 + b \sin\Omega_1 \sin\Omega_2 + c \;, \tag{4.51}$$

for some a, b and c. The expression above can be written as

$$\langle Y \rangle = \frac{a-b}{2}\cos(\Omega_1+\Omega_2) + \frac{a+b}{2}\cos(\Omega_1-\Omega_2) + c \;. \tag{4.52}$$

This shows that the extrema of $\langle Y \rangle$ appears at $\Omega_1 \pm \Omega_2 = 0,\ \pi$ with the corresponding extreme value being

$$\max/\min_{\Omega_1,\Omega_2} \langle Y \rangle = \mp\left(\left|\frac{a-b}{2}\right| + \left|\frac{a+b}{2}\right|\right) + c \;. \tag{4.53}$$

There are two possible solutions. One is $\Omega_1 = \Omega_2 = 0$, which gives $\langle Y \rangle = 1$ and the other is

$$\Omega_1 = \Omega_2 = \frac{\pi}{2} \;. \tag{4.54}$$

In the latter case, the expectation value of Y is simplified to

$$\begin{aligned}\langle Y \rangle = \frac{1}{8}\Bigg(6 + \Big[&\cos\theta_1\cos\theta_2 + \cos\theta_2\cos\theta_3 \\ &+ \cos\theta_3\cos\theta_4 - \cos\theta_4\cos\theta_1\Big] \\ + \Big[&\sin\theta_1\sin\theta_2\cos(\varphi_1-\varphi_2) + \sin\theta_2\sin\theta_3\cos(\varphi_2-\varphi_3) \\ &+ \sin\theta_3\sin\theta_4\cos(\varphi_3-\varphi_4) - \sin\theta_4\sin\theta_1\cos(\varphi_4-\varphi_1)\Big]\Bigg) \;,\end{aligned} \tag{4.55}$$

which depends on 8 angle variables. Let's define 4 unit vectors $\hat{\mathbf{u}}_i$ in 3D real space such that θ_i, φ_i are the corresponding spherical coordinates,

$$\hat{\mathbf{u}}_i = \sin\theta_i(\cos\varphi_i\hat{\mathbf{x}} + \sin\varphi_i\hat{\mathbf{y}}) + \cos\theta_i\hat{\mathbf{z}} \;. \tag{4.56}$$

In that case, the expectation value can be expressed as

$$\langle Y \rangle = \frac{1}{8}\left(6 + \hat{\mathbf{u}}_1\cdot\hat{\mathbf{u}}_2 + \hat{\mathbf{u}}_2\cdot\hat{\mathbf{u}}_3 + \hat{\mathbf{u}}_3\cdot\hat{\mathbf{u}}_4 - \hat{\mathbf{u}}_4\cdot\hat{\mathbf{u}}_1\right) \tag{4.57}$$

At this point, we note that the expression can be written as

$$\langle Y \rangle = \frac{1}{8}\left(6 + \hat{\mathbf{u}}_1\cdot(\hat{\mathbf{u}}_2 - \hat{\mathbf{u}}_4) + \hat{\mathbf{u}}_3\cdot(\hat{\mathbf{u}}_2 + \hat{\mathbf{u}}_4)\right) \tag{4.58}$$

which is more suitable to extremization with respect to $\hat{\mathbf{u}}_1$ and $\hat{\mathbf{u}}_3$. These vectors have to be chosen parallel to the vectors they are multiplied with. Consequently,

$$\min / \max_{\hat{\mathbf{u}}_1,\hat{\mathbf{u}}_3} \langle Y \rangle = \frac{1}{8}\left(6 \mp |\hat{\mathbf{u}}_2 - \hat{\mathbf{u}}_4| \mp |\hat{\mathbf{u}}_2 + \hat{\mathbf{u}}_4|\right) \tag{4.59}$$

Finally, choosing $\hat{\mathbf{u}}_2$ and $\hat{\mathbf{u}}_4$ to be perpendicular to each other gives the extremum values

$$\langle Y \rangle_{\text{min,max}} = \frac{1}{8}(6 \mp 2\sqrt{2}) = \frac{3 \pm \sqrt{2}}{4} \ . \tag{4.60}$$

Summarizing, we find that

$$\Lambda_{\text{sep},min}(Y) = \min_k \Lambda_{\text{sep},min,k}(Y) = 0 \ , \tag{4.61}$$

$$\Lambda_{\text{sep},max}(Y) = \max_k \Lambda_{\text{sep},max,k}(Y) = \frac{3+\sqrt{2}}{4} \approx 1.10355 \ . \tag{4.62}$$

At this point, we notice that the bounds on Y implied by realism arguments is $0 \leq \langle Y \rangle 1$. Therefore, the lower bound coincides. If we express the bounds in terms of the X observable, we get

$$-(1+\sqrt{2}) \leq \langle X \rangle \leq 2 \ . \tag{4.63}$$

4.4 Violation of separability bounds

It is quite straightforward to show that the separability bound $\langle Y \rangle \geq 0$ is violated by a correlated state. The simplest example can be constructed by closely following the violation of CHSH inequality by entangled states. Let

$$|\psi\rangle = \frac{c_1^\dagger c_2^\dagger + c_3^\dagger c_4^\dagger}{\sqrt{2}} |0\rangle \ ,$$

which is clearly a correlated state. The expectation values of number operators and their products are

$$\langle n(\alpha) \rangle = \frac{1}{2} \ , \tag{4.64}$$

$$\langle n(\alpha) n(\beta) \rangle = \frac{1}{2} \left| \alpha_1\beta_2 - \alpha_2\beta_1 + \alpha_3\beta_4 - \alpha_4\beta_3 \right|^2 \ . \tag{4.65}$$

It is appropriate to choose the α orbitals as follows

$$\alpha_1 = \begin{bmatrix} \cos\frac{\theta_1}{2} \\ 0 \\ e^{i\varphi_1}\sin\frac{\theta_1}{2} \\ 0 \end{bmatrix} \qquad \alpha_2 = \begin{bmatrix} 0 \\ \cos\frac{\theta_2}{2} \\ 0 \\ e^{i\varphi_2}\sin\frac{\theta_2}{2} \end{bmatrix} \tag{4.66}$$

$$\alpha_3 = \begin{bmatrix} \cos\frac{\theta_3}{2} \\ 0 \\ e^{i\varphi_3}\sin\frac{\theta_3}{2} \\ 0 \end{bmatrix} \qquad \alpha_4 = \begin{bmatrix} 0 \\ \cos\frac{\theta_4}{2} \\ 0 \\ e^{i\varphi_4}\sin\frac{\theta_4}{2} \end{bmatrix} \tag{4.67}$$

Defining the unit vectors $\hat{\mathbf{u}}_i$ in the same way as in Eq. (4.56), we get

$$\langle Y \rangle = 1 - \frac{1}{4}\left(2 + \hat{\mathbf{u}}_1 \cdot \hat{\mathbf{u}}_2 + \hat{\mathbf{u}}_2 \cdot \hat{\mathbf{u}}_3 + \hat{\mathbf{u}}_3 \cdot \hat{\mathbf{u}}_4 - \hat{\mathbf{u}}_4 \cdot \hat{\mathbf{u}}_1\right) \tag{4.68}$$

Minimization as before gives us the minimum value

$$\langle Y \rangle_{\min} = -\frac{\sqrt{2}-1}{2}\,, \tag{4.69}$$

which is negative. The same example can be used for computing the maximum value

$$\langle Y \rangle_{\max} = \frac{\sqrt{2}+1}{2}\,, \tag{4.70}$$

which can be shown to exceed the bound in Eq. (4.62). Note that these also correspond to $\langle X \rangle$ being $\pm 2\sqrt{2}$. In other words, the maximum violation of separability inequality and the maximum violation of Bell inequality is achieved with the same value of $\langle X \rangle$.

CHAPTER 5

CONCLUSION

This research aimed to find a new outlook on the correlations in many-body systems. In order to do this we have utilized a powerful tool from the quantum information toolkit, namely the witness formalism. Witness formalism has enabled experimentally detection and quantification of quantum entanglement. At the core of the witness formalism is the convexity of the separable states. Separable states form a convex set in the state space. Hyperplane separation theorem states that there exists hyperplanes outside of this convex set separating it from all space. From a physical point of view these hyperplanes correspond to expectation values of observables. However, there are certain conditions for observables to function as witness operators. The seminal works that established the entanglement criteria for 2×2 and 2×3 bipartite states had shown that there are positive but not completely positive maps that have negative eigenvalues for inseparable states. Although this criteria is profound, it is abstract and requires knowledge of the state. Choi-Jamiołkowsky isomorphism rescues the day by pointing out the fact that there exists an operator for every map. This result paved the way for entanglement witness formalism. Witness formalism applies to all dimensions and it is possible to find a witness operator for almost all entanglement scenarios.

The complicated relation between indistinguishability and entanglement has been the subject of many studies. The main challenge comes from the symmetrized or anti-symmetrized wavefunctions of identical particles mathematically appear like entangled states. This coincidence has been treated with different approaches. Although, it is difficult to announce a consensus on the matter, from quantum information point of view any meaningful entanglement definition should fall within the LOCC paradigm, which means entanglement cannot increase under local operations and classical communications.

Equipped with all the necessary tools and concepts mentioned above in Chp.2 from quantum information we introduced witness for pairing correlations in Chp 3. In order to do so, we first defined the set of separable states for both fermions and bosons. The results for fermions matches with [46], however there is no bosonic counterpart for witnessing pairing correlations in the literature. In this study this gap is filled. For bosonic pairing we defined two kinds of unpaired states, and named them type-1 and type-2 product states. The main idea is to compare the largest eigenvalue to largest separability bound. A straightforward calculation for the separability bound for type-1 states was possible, unfortunately an analytical result for type-2 separability bounds could not be found. Instead numerical results were shown.

In the same spirit of adopting witness formalism we have adopted Bell-type operators for a fermionic set up in Chp. 4. Originally Bell-type operators provide a test for non-locality. In this case we do not claim a non-locality inequality but one for the correlation among fermionic number states. First a CHSH inequality with a fermionic dichotomic number operators is established, then the separability bounds are found and finally it is shown that these bounds can be violated. Adopting a CHSH test in the fermionic and bosonic Fock space could produce interesting results.

One of the triumphs of pairing is to expose a macroscopic effect, that is superconductivity, which has no classical explanation. Physical consequences of pairing correlations, thus, may be seen at the macroscopic boundaries of quantum mechanics. It's not meaningless to assume pairing correlations exist in almost every many-particle systems. Although, observing the effects of pairing or its significance at that matter is another subject. The idea behind this work which is adopting quantum information toolkit to many-body systems is attracting more interest and becoming a part of condensed matter physics [50].

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APPENDIX A

SEPARABILITY BOUND FOR TYPE 1 PRODUCT STATES

Type-1 product states were already defined in Eq. (3.18). First, the expectation value of $Q^\dagger Q$ will be simplified. Begin with rewriting type-1 product states,

$$|\Psi\rangle_{type-1} = \frac{(b^\dagger(\alpha_1))^{m_1}}{\sqrt{m_1!}} \cdots \frac{(b^\dagger(\alpha_p))^{m_p}}{\sqrt{m_p!}} |0\rangle = |m_1, m_2, \ldots, m_p\rangle \ ,$$

where $b^\dagger(\alpha_\lambda) = \sum \alpha_{\lambda i} c_i^\dagger$ and $Q = \frac{1}{2}\sum_{i=1}^r c_i^2$ operators for bosons. Now, note that

$$\begin{aligned} \left\langle Q^\dagger Q \right\rangle &= \langle \Psi | Q^\dagger Q | \Psi \rangle \\ &= ||Q\,|\Psi\rangle\,||^2 \ . \end{aligned}$$

We only need to compute $Q\,|\Psi\rangle$. Now using the commutation relation $\left[c_i, b^\dagger(\alpha_\lambda)\right] = \alpha_{\lambda i}$, we can show that;

$$\langle Q^\dagger Q\rangle_\Psi = \sum_{a<b} |R_{ab}|^2 m_a m_b + \sum_a \frac{1}{4} |R_{aa}|^2 m_a (m_a - 1) \ , \tag{A.1}$$

where

$$R_{a,b} = \sum_{i=1}^r \alpha_{a,i}\alpha_{b,i} \ , \tag{A.2}$$

and m_a are positive integers that satisfy $\sum_a m_a = N$. R_{ab} can be expressed as $R_{ab} = R_{ba} = \langle \alpha_a^* | P | \alpha_b \rangle$, i.e., the overlap between α_a^* and α_b on the subspace corresponding to *ad hoc* single particle states, where P is the projection onto the said subspace which is the space spanned by the first r single-particle states. Let define $D_{ab} = |R_{ab}|^2$. Note that D_{ab} is a $p \times p$, symmetric, doubly substochastic matrix, i.e.,

$$\sum_{b=1}^p D_{ab} \leq 1 \ .$$

Now, we can express the expectation value $\left\langle Q^\dagger Q \right\rangle$ as a linear function of the elements of D as follows;

$$f(D) \equiv \frac{1}{2} \sum_{a \neq b} D_{ab} m_a m_b + \frac{1}{4} \sum_a D_{aa} m_a (m_a - 1) \ . \tag{A.3}$$

A direct approach to maximization problem would follow in two steps: First maximize over the set of D matrices then maximize over the number of particles m_a. Unfortunately, this is not possible due to restrictions $D_{ab} = |R_{ab}|^2$ along with Eq. (A.2). To remedy this situation; assume that $f(D)$ has a maximum over the *whole set* of substochastic matrices and there is a D matrix that yields this maximum and satisfies the restrictions mentioned before.

D matrices are doubly-stochastic matrices with non-negative elements,i.e. $\sum_b D_{ab} = \sum_b D_{ba} = 1$. Birkhoff's theorem [39] states that extreme points of the set of doubly-stochastic matrices (which is a convex set) are *permutation matrices*. Therefore, since the function $f(D)$ is maximized at these extreme points, it is maximized by a permutation matrix D.Permutation matrices have single entry 1 at each row and column.

Now, it will be shown that the D matrices with 2-cycle structures produce the maximization of $f(D)$. Suppose that D has an ℓ-cycle structure then there will be terms of

$$\frac{1}{2}\left(m_1 m_2 + m_2 m_3 + \cdots + m_\ell m_1\right) \tag{A.4}$$

in Eq. (A.3). Note that a relabeling is implied. So that, for $\ell \geq 5$ there will be a term $m_1 m_2 + m_2 m_3 + m_3 m_4 + m_4 m_5 + m_\ell m_1$. If two different pairs of labels are let to conjoin then the ℓ-cycle can be replaced by an $(\ell - 2)$-cycle thus this increases $f(D)$, which can be seen from

$$\begin{aligned} &m_\ell m_1 + m_1 m_2 + m_2 m_3 + m_3 m_4 + m_4 m_5 \\ &\qquad < m_\ell(m_1 + m_3) + (m_1 + m_3)(m_2 + m_4) + (m_2 + m_4)m_5 \,. \end{aligned} \tag{A.5}$$

Similarly 4-cycle and 3-cycle permutations can be replaced by a 2-cycle permutation by making the observations;

$$\frac{1}{2}(m_1 m_2 + m_2 m_3 + m_3 m_4 + m_4 m_1) < (m_1 + m_3)(m_2 + m_4)\,, \tag{A.6}$$

$$\frac{1}{2}\left(m_1 m_2 + m_2 m_3 + m_3 m_1\right) < m_1(m_2 + m_3)\,, \tag{A.7}$$

for the latter case $m_1 \geq m_2, m_3$ is required. Consequently, the maximum is attained at $p = 2$ orbitals with the corresponding matrices

$$D = R = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \,. \tag{A.8}$$

This result suggests that $\langle \alpha_1^* | \alpha_2 \rangle = \langle \alpha_2^* | \alpha_1 \rangle = 1$, and $\alpha_2^* = \alpha_1$, $\alpha_1^* = \alpha_2$. Each α single-particle orbitals are superposition of the first r basis states.

Finally, it can be seen that

$$\Lambda_{r,N}^{\mathrm{sep(type1)}} = \max_{m_1+m_2=N} m_1 m_2 \tag{A.9}$$

$$= \begin{cases} \frac{N^2}{4} & \text{if } N \text{ is even} \\ \frac{N^2-1}{4} & \text{if } N \text{ is odd} \end{cases} \tag{A.10}$$

Since the number of single-particle states is $p = 2$, the rank of Q operators r does not change this result as long as $r \geq 2$.

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