# Pairing in fermionic systems: A quantum-information perspective

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The notion of "paired" fermions is central to important condensed-matter phenomena such as superconductivity and superfluidity. While the concept is widely used and its physical meaning is clear, there exists no systematic and mathematical theory of pairing that would allow us to unambiguously characterize and systematically detect paired states. We propose a definition of pairing and develop methods for its detection and quantification applicable to current experimental setups. Pairing is shown to be a quantum correlation different from entanglement, giving further understanding in the structure of highly correlated quantum systems. In addition, we will show the resource character of paired states for precision metrology, proving that the BCS states allow phase measurements at the Heisenberg limit.

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## I. INTRODUCTION

The notion of pairing in fermionic systems is at least as old as the seminal work of Bardeen, Cooper, and Schrieffer explaining superconductivity [1]. The formation of fermionic pairs with opposite spin and momentum is not only the source for the vanishing resistance in solid-state systems, but it can also explain many other interesting phenomena, like superfluidity in helium-3 or inside a neutron star.

For instance, with recent progress in the field of ultracold quantum gases, fermionic pairing has gained again a lot of attention [2–9]. These experiments allow an excellent control over many parameters inherent to the system, offering a unique testing ground for existing theories and an exploration of new and exotic phases. However, the notion of pairing in these systems is less clear and sometimes even controversial. Recent experiments on the BEC-BCS crossover have caused a heated debate over whether the obtained data were in agreement with pairing [7,10–12]. In addition, pairing without superfluidity [13] has been observed in these experiments, raising fundamental questions on quantum correlations in fermionic many-body systems.

Motivated by these exciting experiments and the central role pairing plays in many physical phenomena, and by the perceived lack of accepted criteria to verify the presence of pairing in a quantum state, we propose a clear and unambiguous definition of pairing intended to capture its two-particle nature and to allow a systematic study of the set of paired states and its properties. We employ methods and tools from quantum-information theory to gain a better understanding of the set of fermionic states that display pairing. In particular, we develop tools for the systematic detection and for the quantification of pairing, which are applicable to current experiments. Our approach is inspired by concepts and methods from entanglement theory, thus building a bridge between quantum-information science and condensed-matter physics.

Since they contain nontrivial quantum correlations, paired states belong to the set of entangled many-body states. However, pairing will turn out to be not equivalent to any known concept of entanglement in systems of indistinguishable particles [14–29] but to represent a particular type of quantum correlation of its own. We will show that these correlations can be exploited for quantum-phase estimation. Hence pairing constitutes a resource in state estimation using fermions as much as entangled states with spins.

This paper is organized as follows. After the introduction of the language necessary for the description of fermionic systems in Sec. II, we will introduce the general framework of pairing theory in Sec. III. This part includes our definition of pairing and methods for its detection and quantification. In order to validate the theory, we will apply it to two different classes of fermionic states in Secs. IV and V. We start out with pairing in fermionic Gaussian states in Sec. IV. The interest in this family of states is twofold. First, the pairing problem can be solved completely in this case, so that Gaussian states are particularly interesting from a conceptual point of view. Second, there exists a relation between pure fermionic Gaussian states and the BCS states of superconductivity (see Sec. II D for the details), which are examples of paired states par excellence. This enables us to translate methods developed for the detection and quantification of pairing for Gaussian states to the BCS states. The reader interested in the application of our pairing theory to experimental application is referred to Sec. V. There we study pairing for number-conserving states, i.e., states commuting with the number operator. This class includes the states appearing in the BEC-BCS crossover, and we will develop tools for the detection of pairing tailored for these systems. In Sec. VI, we will show that certain classes of paired states constitute a resource for quantum-phase estimation, proving that pairing is a resource similar to entanglement.

## II. FERMIONIC STATES

In this section, we review the basic concepts needed for the understanding of fermionic systems. We start out with some notation used for the description of fermionic systems in second quantization in Sec. II A. As pairing is a special sort of correlation, we continue with a review on quantum correlations and entanglement in systems of indistinguishable particles in Sec. II B. This general part is followed by the introduction of fermionic Gaussian states and number-conserving states in Secs. II C and II D. The latter includes the introduction of BCS states and their relation to the Gaussian states. As this part is only necessary for the application of the pairing theory to these concrete examples in Secs. IV and V, it is possible to skip this part at the beginning, and then refer to it later on.

### A. Basic notation

We consider fermions on an $M$-dimensional single-particle Hilbert space $\mathcal{H}=\mathbb{C}^M$. All observables are generated by the creation and annihilation operators $a_j^\dagger$ and $a_j$, $j=1,\dots,M$, which satisfy the canonical anticommutation relations (CAR) $\{a_k,a_l\}=0$ and $\{a_k,a_l^\dagger\}=\delta_{kl}$. We say $a_j^\dagger$ creates a particle in mode (or single-particle state) $e_j$, where $\{e_j\}\subset\mathbb{C}^M$ denotes the canonical orthonormal basis of $\mathcal{H}$. In general, for any normalized $f\in\mathcal{H}$, we define $a_f\equiv\Sigma_k f_j a_j$, the annihilation operator for mode $f$.

Sometimes a description using the $2M$ Hermitian Majorana operators $c_{2j-1}=a_j^\dagger+a_j$, $c_{2j}=(-i)(a_j^\dagger-a_j)$, which satisfy $\{c_k,c_l\}=2\delta_{kl}$, is more convenient.

The Hilbert space of the many-body system, the antisymmetric Fock space over $M$ modes, $\mathcal{A}_M$, is spanned by the orthonormal Fock basis defined by

$$|n_1,\dots,n_M\rangle=(a_1^\dagger)^{n_1}\cdots(a_M^\dagger)^{n_M}|0\rangle, \tag{1}$$

where the vacuum state $|0\rangle$ fulfills $a_j|0\rangle=0\ \forall\ j$. The $n_j\in\{0,1\}$ are the eigenvalues of the mode occupation number operators $n_j=a_j^\dagger a_j$. The $N$-particle subspace spanned by vectors of the form (1) satisfying $\Sigma_i n_i=N$ is denoted by $\mathcal{A}_M^{(N)}$. The set of density operators on the Hilbert space $\mathcal{H}=\mathcal{A}_M,\mathcal{A}_M^{(N)}$ is denoted by $\mathcal{S}(\mathcal{H})$.

Linear transformations of the fermionic operators which preserve the CAR are called canonical transformations. They are of the form $c_k\mapsto c_k'=\Sigma_l O_{kl}c_l$, where $O\in O(2M)$ is an element of the real orthogonal group. These transformations can be implemented by unitary operations $U_O$ on $\mathcal{A}_M$ which are (for det $O=1$) generated by quadratic Hamiltonians in the $c_j$ (see, e.g., [30]). The subclass of canonical operations that commute with the total particle number $N_{\text{op}}=\Sigma_i n_i$ are called passive transformations. They take a particularly simple form in the complex representation $a_k\mapsto a_k'=\Sigma_l U_{kl}a_l$, where $U$ is unitary on the single-particle Hilbert space $\mathcal{H}$, i.e., they describe (quasi)free time evolution of independent particles. Canonical transformations that do not commute with $N_{\text{op}}$ are called active. They mix creation and annihilation operators.

### B. Quantum correlations of fermionic states

The notion of "pairing" used in the description of superconducting solids, superfluid liquids, baryons in nuclei, etc. is always associated with a correlated fermionic system. The subject of quantum correlations in fermionic systems is vast (see [31], and for instance [32–34]). In recent years, there has been renewed interest from the perspective of quantum-information theory. There quantum correlations (also known as entanglement) of distinguishable systems (qubits) play a crucial role as a resource enabling certain state transformations or information-processing tasks. The detailed quantitative analysis of quantum correlations motivated by this has proven to be valuable also in the understanding of condensed-matter systems (see [35] for a review).

In contrast to the usual quantum-information setting, which studies the entanglement of distinguishable particles, the indistinguishable nature of the fermions is of utmost importance in the settings of our interest. The existing concepts for categorizing entanglement in systems of indistinguishable particles fall into two big classes: Entanglement of modes [14–22] and entanglement of particles. Entanglement of particles has been considered, e.g., in [23–29], leading to the concept of Slater rank [24,25], being the generalization of the Schmidt rank to indistinguishable particles. We show in Sec. III that our definition of pairing does not coincide with any of the existing ideas. We refrain from giving an exhaustive review on the existing concepts, referring the interested reader to the mentioned literature and references therein, and we restrict ourselves to the following definition:

*Definition II.1.* A pure fermionic state $\rho_p^{(N)}=|\Psi_p^{(N)}\rangle\langle\Psi_p^{(N)}|\in\mathcal{S}(\mathcal{A}_M^{(N)})$ is called a *product state*, if there exists a passive transformation $a_k\mapsto a_k'$ such that

$$|\Psi_p^{(N)}\rangle=\prod_{j=1}^{N}a_j'^{\dagger}|0\rangle. \tag{2}$$

A state $\rho_s$ is called *separable*, if it can be written as the convex combination of product states, i.e.,

$$\rho_s=\sum_{p=1}^{K}\lambda_p\rho_p^{(N_p)}, \tag{3}$$

where $\Sigma_{p=1}^K\lambda_p=1$, $\lambda_p\geqslant 0$ and all $\rho_p^{(N_p)}\in\mathcal{S}(\mathcal{A}_M^{(N_p)})$ are product states. All other states are said to have "Slater number larger than 1" and are called *entangled* (in the sense of [24,25]).

We denote the set of all separable states by $\mathcal{S}_{\text{sep}}$ and by $\mathcal{S}_{\text{sep}}^{(N)}\equiv\mathcal{S}_{\text{sep}}\cap\mathcal{S}(\mathcal{A}_M^{(N)})$ the set of all separable states of particle number $N$.

Note that the sets $\mathcal{S}_{\text{sep}}$, $\mathcal{S}_{\text{sep}}^{(N)}$ of separable states are convex and invariant under passive transformations. Both properties will be useful later on.

Separable states have only correlations resulting from their antisymmetric nature and classical correlations due to mixing. In the terminology of Refs. [24,25], they have Slater number one and describe unentangled particles. These states will certainly not contain correlations associated with pairing. (Note that they can be mode-entangled for an appropriate partition of modes.)

Besides basis change, there are other operations that do not create quantum correlations, and it is useful to see that the set of separable states is invariant under them.

*Lemma II.2.* Let $\rho\in\mathcal{S}_{\text{sep}}$ be a separable state. Then the state after measuring the particle number $n_h=a_h^\dagger a_h$ in some mode $h$ is separable for both possible outcomes $n_h=0,1$. Furthermore, $\rho_h\equiv\text{tr}_{a_h}[\rho]$, the reduced state obtained by tracing out the mode $a_h$, is also separable.

*Proof.* As $\mathcal{S}_{\text{sep}}$ is convex, it is sufficient to prove the claim for product states $\rho$. Let $|\Psi\rangle=\Pi_{j=1}^N a_{f_j}^\dagger|0\rangle$ be the vector in Hilbert space corresponding to $\rho$. Our aim is to show that $|\Psi\rangle$

$=|\Psi_0\rangle+|\Psi_1\rangle$, where $|\Psi_l\rangle$ are product states and $n_h=l$ eigenstates of the occupation number operator $n_h$. If $h$ is in the span of $\{f_{1\leq k\leq N}\}$ or orthogonal to it, the state already is an $n_h$ eigenstate and we are done. Otherwise, define $f_{N+1}$ orthogonal to the $f_{k\leq N}$ such that $h\in\text{span}\{f_{1\leq k\leq N+1}\}$ and define another orthonormal basis $\{g_j\}$ for the span with $g_1=h$ and $g_2\propto f_{N+1}-(hf_{N+1})h$ [here $(hf_{N+1})$ denotes the inner product on the single-particle Hilbert space]. Then we can write $|\Psi\rangle=a_{f_{N+1}}a^\dagger_{f_{N+1}}\Pi_{j=1}^{N}a^\dagger_{f_j}|0\rangle=(xa_{g_1}+ya_{g_2})\Pi_{j=1}^{N+1}a^\dagger_{g_j}|0\rangle$ for some $x,y\in\mathbb{C}$. Hence, $|\Psi\rangle=|\Psi_0\rangle+|\Psi_1\rangle$ with $|\Psi_0\rangle=x\Pi_{j=2}^{N+1}a^\dagger_{g_j}|0\rangle$ and $|\Psi_1\rangle=-ya^\dagger_h\Pi_{j=3}^{N+1}a^\dagger_{g_j}|0\rangle$, which both clearly are product states. The reduced state $\text{tr}_h[|\Psi\rangle\langle\Psi|]$ is the statistical mixture of $|\Psi_0\rangle$ and $|\Psi_1\rangle$ and therefore clearly separable. ■

### C. Fermionic Gaussian states

Fermionic Gaussian states are represented by density operators that are exponentials of a quadratic form in the Majorana operators. A general multimode Gaussian state is of the form

$$\rho=K\exp\left[-\frac{i}{4}c^TGc\right], \tag{4}$$

where $c=(c_1,\dots,c_{2M})$, $K$ is a normalization constant, and $G$ is a real antisymmetric $2M\times 2M$ matrix. Every antisymmetric matrix can be brought to a block-diagonal form

$$OGO^T=\bigoplus_{j=1}^{M}\begin{pmatrix}0 & -\beta_j\\ \beta_j & 0\end{pmatrix} \tag{5}$$

by a special orthogonal matrix $O\in\text{SO}(2M)$.

From Eq. (4), it is clear that Gaussian states have an interpretation as thermal (Gibbs) states corresponding to a Hamiltonian $H$ that is a quadratic form in the $c_k$, i.e., $H=\frac{i}{4}c^TGc=\frac{i}{4}\Sigma_{k>l}G_{kl}[c_k,c_l]$, and the form Eq. (5) shows that every Gaussian state has a normal-mode decomposition in terms of $M$ single-mode "thermal states" of the form $\sim\exp(-\beta a^\dagger a)$. From this one can see that the state is fully determined by the expectation values of quadratic operators $a_ia_j$ and $a_i^\dagger a_j$. These are collected in a convenient form in the real and antisymmetric covariance matrix $\Gamma$, which is defined via

$$\Gamma_{kl}=\frac{i}{2}\text{tr}(\rho[c_k,c_l]). \tag{6}$$

It can be brought into block-diagonal form by a canonical transformation,

$$O\Gamma O^T=\bigoplus_{i=1}^{M}\begin{pmatrix}0 & \lambda_j\\ -\lambda_j & 0\end{pmatrix}. \tag{7}$$

For every valid density operator, $\lambda_j\in[-1,1]$, and the eigenvalues of $\Gamma$ are given by $\pm i\lambda_j$. Hence, every $\Gamma$ corresponding to a physical state has to fulfill $i\Gamma\leq\mathbb{1}$ or, equivalently, $\Gamma\Gamma^\dagger\leq\mathbb{1}$, and to each such $\Gamma$ corresponds a valid Gaussian density operator where the relation between $G$ and $\Gamma$ is given by $\lambda_j=\tanh(\beta_j/2)$. The covariance matrix of the ground state of $H$ is obtained in the limit $|\beta_j|\to\infty$, i.e., $\lambda_j\to\text{sgn}(\beta_j)$. In fact, this shows that every pure Gaussian state is the ground state to some quadratic Hamiltonian. The purity of the state can be easily determined from the covariance matrix as a Gaussian state is pure if and only if $\Gamma^2=-\mathbb{1}$ (see, e.g., [36]).

As mentioned, Gaussian states are fully characterized by their covariance matrix and all higher correlations can be obtained from $\Gamma$ by Wick's theorem (see, e.g., [36]) via

$$i^p\text{tr}[\rho c_{j_1}\cdots c_{j_{2p}}]=\text{Pf}(\Gamma_{j_1,\dots,j_{2p}}), \tag{8}$$

where $1\leq j_1<\cdots<j_{2p}\leq 2M$ and $\Gamma_{j_1,\dots,j_{2p}}$ is the corresponding $2p\times 2p$ submatrix of $\Gamma$. $\text{Pf}(\Gamma_{j_1,\dots,j_{2p}})^2=\det(\Gamma_{j_1,\dots,j_{2p}})$ is called the Pfaffian.

In some cases it is more appropriate to use a different ordering of the Majorana operators, the so-called *q-p* ordering $c=(c_1,c_3,\dots,c_{2M-1};c_2,c_4,\dots,c_{2M})$, opposed to the mode-ordering introduced at the beginning. When using the *q-p* ordering, the relation between the real and complex representation is given by

$$c^T=\Omega a^T,\quad \Omega=\begin{pmatrix}\mathbb{1} & \mathbb{1}\\ i\mathbb{1} & -i\mathbb{1}\end{pmatrix}, \tag{9}$$

where $a=(a_1,\dots,a_M,a_1^\dagger,\dots,a_M^\dagger)$. The transformation matrix $\Omega$ fulfills $\Omega\Omega^\dagger=2\mathbb{1}$.

In the *q-p* ordering, the covariance matrix obtains the following block structure:

$$\tilde{\Gamma}=\begin{pmatrix}\Gamma_q & \Gamma_{qp}\\ -\Gamma_{qp}^T & \Gamma_p\end{pmatrix}. \tag{10}$$

Finally, for some purposes it is more convenient to use the complex representation, where the covariance matrix is of the form

$$\Gamma_c=\frac{1}{4}\Omega^\dagger\tilde{\Gamma}\bar{\Omega}=\begin{pmatrix}Q & R\\ \bar{R} & \bar{Q}\end{pmatrix}, \tag{11}$$

where $Q_{kl}=\langle i/2[a_k,a_l]\rangle$, $R_{kl}=\langle i/2[a_k,a_l^\dagger]\rangle$, and $\bar{Q}$ denotes the complex conjugate. Note that $R^\dagger=-R$ and $Q^T=-Q$ and hence $\Gamma_c^T=-\Gamma_c$. The condition $\tilde{\Gamma}\tilde{\Gamma}^\dagger\leq\mathbb{1}$ takes the form $4\Gamma_c\Gamma_c^\dagger\leq\mathbb{1}$.

The description of $\rho$ by its covariance matrix is especially convenient to describe the effect of canonical transformations, i.e., time evolutions generated by quadratic Hamiltonians: if $c_k\mapsto\Sigma_lO_{kl}c_l$ in the Heisenberg picture, then $\Gamma\mapsto O\Gamma O^T$ in the Schrödinger picture. For a passive transformation $a_k\mapsto a_k'=\Sigma_lU_{kl}a_l$, the *q-p*-ordered Majorana operators transform as

$$c^T\mapsto c'^T=O_pc^T,\quad O_p=\begin{pmatrix}X & Y\\ -Y & X\end{pmatrix}, \tag{12}$$

where $X=\text{Re}(U)$ is the real part of the unitary $U$, and $Y=\text{Im}(U)$ is the imaginary part. Note that $O_p$ is both orthogonal and symplectic. The behavior of $\Gamma_c$ under a passive transformation is particularly simple: $Q$ and $R$ transform according to $Q\mapsto UQU^T$ and $R\mapsto URU^\dagger$.

Passive transformations can be used to transform *pure* fermionic states to a simple standard form, the so-called Bloch-Messiah reduction [37]. The *q-p*-ordered CM $\tilde{\Gamma}_{\text{BCS}}$ takes the form (10), where

$$\Gamma_q = -\Gamma_p = \bigoplus_k \begin{pmatrix} 0 & -2\,\mathrm{Im}(u_k v_k^*) \\ 2\,\mathrm{Im}(u_k v_k^*) & 0 \end{pmatrix}, \quad (13)$$

$$\Gamma_{qp} = \bigoplus_k \begin{pmatrix} |u_k|^2 - |v_k|^2 & 2\,\mathrm{Re}(u_k v_k^*) \\ -2\,\mathrm{Re}(u_k v_k^*) & |u_k|^2 - |v_k|^2 \end{pmatrix}. \quad (14)$$

In Hilbert space, the state in standard form is given by

$$|\Psi_{\mathrm{Gauss}}^{(\bar{N})}\rangle = \prod_k (u_k + v_k a_k^\dagger a_{-k}^\dagger)|0\rangle, \quad (15)$$

where $u_k, v_k \in \mathbb{C}$, $|u_k|^2+|v_k|^2=1$, and $\bar{N}=\Sigma_k\langle a_k^\dagger a_k\rangle = 2\Sigma_k|v_k|^2$. This comprises the kind of "paired" states appearing in the BCS theory of superconductivity [1] with $k\equiv(\vec{k},\uparrow)$, $-k \equiv(-\vec{k},\downarrow)$. We will refer to these states as *Gaussian BCS states*. We would like to stress the fact that every pure Gaussian state is a Gaussian BCS state in some basis.

### D. Number-conserving fermionic states

For the application to physical systems, we are interested in states for which the particle number is a conserved quantity. We call $\rho$ a number-conserving state if $[\rho, N_{\mathrm{op}}]=0$, where $N_{\mathrm{op}}$ denotes the total number operator. Thus, the density operator of a number-conserving state can be written as a mixture of $N_{\mathrm{op}}$ eigenstates. In particular, all separable states as defined in Def. II.1 are number-conserving.

The Gaussian BCS wave function (15) is not number-conserving (except for the case $\Sigma_k|u_k v_k|=0$ that either $u_k$ or $v_k$ vanishes for every mode), but a relation to these states can be established via the identity

$$|\Psi_{\mathrm{Gauss}}^{(\bar{N})}\rangle = \sum_{N=0}^{2M} \lambda_N |\Psi_{\mathrm{BCS}}^{(N)}\rangle, \quad (16)$$

where the number-conserving $2N$-particle BCS state is given by

$$|\Psi_{\mathrm{BCS}}^{(N)}\rangle = C_N\left(\sum_{k=1}^{M} \alpha_k P_k^\dagger\right)^N |0\rangle, \quad (17)$$

where we have introduced the pair creation operator $P_k^\dagger = a_k^\dagger a_{-k}^\dagger$. The coefficients $\alpha_k$ are related to $u_k$ and $v_k$ via $\alpha_k = v_k/u_k$, and $C_N$ is a normalization constant, which is seen to be

$$C_N = \left((N!)^2 \sum_{j_1<\cdots<j_N} |\alpha_{j_1}|^2 \cdots |\alpha_{j_N}|^2\right)^{-1/2}$$

by rewriting Eq. (17) as

$$C_N N! \sum_{j_1<j_2<\ldots<j_N} \alpha_{k_1}\cdots\alpha_{k_N} P_{k_1}^\dagger \cdots P_{k_N}^\dagger|0\rangle. \quad (18)$$

The coefficients $\lambda_N = (\Pi_k u_k)/(N! C_N)$ can be interpreted as the probability amplitude of being in state $|\Psi_{\mathrm{BCS}}^{(N)}\rangle$ since $\Sigma_N|\lambda_N|^2=1$. We will in general drop the term *number-conserving* and refer to states of the form (17) as *BCS states*.

Whenever the distribution of the $\lambda_N$ is sharply peaked around some average particle number $\bar{N}$, expectation values of relevant observables for the number-conserving BCS states $|\Psi_{\mathrm{BCS}}^{(\bar{N})}\rangle$ are approximated well by the expectation values of the Gaussian BCS state. This relation will turn out to be very useful later on, as results on Gaussian states can be translated into results on number-conserving BCS states.

## III. PAIRING THEORY

In this section, we introduce a precise definition of pairing as a property of quantum states.

### A. Motivation and statement of the definition

The simplest system in which we can find pairing consists of two particles and four modes.[1] The prototypical paired state, for example the spin-singlet of two electrons with opposing momenta, is of the form

$$|\Phi\rangle = \frac{1}{\sqrt{2}}(a_1^\dagger a_2^\dagger + a_3^\dagger a_4^\dagger)|0\rangle. \quad (19)$$

The states describing many Cooper pairs in BCS theory are generalizations of $|\Phi\rangle$.

The state $|\Phi\rangle$ describes correlations between the two particles that cannot be reproduced by any uncorrelated state, and it can be completely characterized by one- and two-particle expectations (consisting of no more than two creation and annihilation operators each). This is a characteristic of the two-particle property "pairing" that we propose to make the central *defining* property of paired states in the general case of many modes, many particles, and mixed states. Since, moreover, we would call the state $|\Phi\rangle$ paired no matter what basis the mode operators $a_i$ refer to and we want it to comprise all BCS states, we are led to the following list of requirements that a sensible definition of pairing should fulfill:

(i) States that have no internal quantum correlation must be unpaired. These are the separable states (3).

(ii) Pairing must reveal itself by properties related to one- and two-particle expectations only.

(iii) Pairing should be a basis-independent property.

(iv) The standard "paired" states appearing in the description of solid-state and condensed-matter systems, i.e., the BCS states with wave function (17), must be captured by our definition.

Further, it would be desirable that there exist examples of paired states that are a resource for some quantum-information application.

Let us define the following:

*Definition III.1*. The set of all operators $\{O_\alpha\}_\alpha$ on $\mathcal{A}_M$, which are the product of at most two creation and two annihilation operators, is called the set of *two-particle operators*. We denote it by $A_2$.

These operators capture all one- and two-particle properties of a state $\rho$ and should therefore contain all information about pairing. We will call a state $\rho$ paired if it can be distinguished from separable states by looking at observables in

[1] For three modes, all pure two-particle states are of product form.

$A_2$ alone. This is formalized in the following definition:

*Definition III.2*. A fermionic state $\rho$ is called *paired* if there exists a set of operators $\{O_\alpha\}_\alpha \subseteq A_2$ such that the expectation values $\{\mathrm{tr}[\rho O_\alpha]\}$ cannot be reproduced by any separable state $\rho_s \in \mathcal{S}_{\rm sep}$. States that are not paired are called *unpaired*.

This definition automatically fulfills our first two requirements by definition. The third, basis independence, clearly holds, since the set of separable states is invariant under passive transformations. We will show that the last requirement is met, both for Gaussian and number-conserving BCS states, i.e., all of them are paired (see Lemma V.3 and Sec. IV B). Moreover, in Sec. VI we can show that there exist paired states that are a resource for quantum metrology.

For states with a fixed particle number, i.e., $\rho \in \mathcal{S}(\mathcal{A}_M^{(N)})$, it is sufficient to compare with expectation values on $N$-particle separable states $\rho_s^{(N)} \in \mathcal{S}_{\rm sep}^{(N)}$, as for all other states the expectation values of $\langle \Sigma_i n_i\rangle$ and $\langle (\Sigma_i n_i)^2\rangle$ differ due to the particle number constraint. For number-conserving states, only number-conserving observables lead to nonvanishing expectation values and one can thus restrict to linear combinations of $a_i^\dagger a_j$, $a_i^\dagger a_j^\dagger a_k a_l$.

For Gaussian states, pairing must reveal itself by properties of the covariance matrix, as all higher correlations can be obtained from it via Eq. (8). This important fact enables us to give a complete solution of the pairing problem for fermionic Gaussian states, which we present in Sec. IV.

### B. Relation of pairing and entanglement

Paired states are fermionic states exhibiting nontrivial quantum correlations. In particular, by definition paired states are inseparable, i.e., entangled in the sense of [24,25]. This raises immediately the following question: Is pairing equivalent to entanglement? Below, we provide examples of entangled but unpaired states that demonstrate that pairing is not equivalent to entanglement (of particles) but represents a special type of quantum correlation.[2]

*Lemma III.3*. There exist states that are entangled according to the Slater rank concept, but not paired.

*Proof*. Consider the state $|\Psi_4\rangle = \frac{1}{2}(a_1^\dagger a_2^\dagger a_3^\dagger a_4^\dagger + a_5^\dagger a_6^\dagger a_7^\dagger a_8^\dagger)|0\rangle$, which is entangled according to the Slater rank definition. However, one sees immediately that the one- and two-particle expectations for $|\Psi_4\rangle$ are the same as for $\rho_s^{(4)} = \frac{1}{2}|\Phi_1\rangle\langle\Phi_1| + \frac{1}{2}|\Phi_2\rangle\langle\Phi_2|$, where $|\Phi_1\rangle = a_1^\dagger a_2^\dagger a_3^\dagger a_4^\dagger|0\rangle$, $|\Phi_2\rangle = a_5^\dagger a_6^\dagger a_7^\dagger a_8^\dagger|0\rangle$. Since $\rho_s^{(4)}$ is a product state, $|\Psi_4\rangle$ is not paired. One can construct further examples in a similar manner using, e.g., other states with higher Slater rank. ∎

Since pairing is defined via expectation values of one- and two-particle operators only, one might wonder whether pairing is related to entanglement of the two-particle reduced state. To study this relation, we recall the definition of the *two-particle density operator* and the closely related *two-particle density matrix* (see, e.g., [38]):

*Definition III.4*. Let $\rho$ be the density operator of a fermionic state. Then $O^{(\rho)}_{(ij)(kl)} = \mathrm{tr}[\rho a_i^\dagger a_j^\dagger a_l a_k]$ is called the *two-particle reduced density matrix* (RDM). It is usually not normalized and fulfills $\mathrm{tr}[O^{(\rho)}] = \langle N_{\rm op}^2\rangle - \langle N_{\rm op}\rangle$. The operator $\rho_2 = O^{(\rho)}/\mathrm{tr}[O^{(\rho)}]$ is called the *reduced two-particle density operator* (RDO).

Note the crucial difference between the two-particle RDM and the RDO. While the RDM contains all two-particle correlations of $\rho$, the RDO corresponds to the two-particle state of any two particles when the rest of the system is discarded. We would like to emphasize that pairing is *not* equivalent to entanglement of the RDO, and therefore it is a property of the one- and two-particle expectations:

*Lemma III.5*. Let $|\Psi_{\rm BCS}^{(N)}\rangle$ be a number-conserving BCS state as defined in Eq. (17) with $\alpha_k = 1\ \forall\, k = 1, \ldots, M$. Then its two-particle RDO (see Def. III.4) $\rho_{\rm BCS,2}^{(N)}$ is always paired. However, $\rho_{\rm BCS,2}^{(N)}$ is entangled if and only if $M > 3N-2$.

The proof is given in Appendix E.

We would like to stress the point that Lemma III.5 shows the existence of paired states that are not entangled. Having assured that our definition of pairing does not coincide with entanglement, we now turn to methods of detecting and quantifying pairing.

### C. Methods for detecting pairing

Taking Def. III.2, we aim at finding tools that can be used for the detection and quantification of pairing. These will be applied to systems of Gaussian states and number-conserving states in Secs. IV and V, respectively. In this section, we exploit the convexity of the set of unpaired states to introduce witness operators and obtain a geometrical picture of the set. The quantification of pairing via pairing measures will be discussed in Sec. III D.

Given a fermionic density operator, we are interested in an operational method to determine whether it is paired or not. As in the case of separability, this simple-sounding question will turn out to be rather difficult to answer in general.

Starting from Def. III.2, it is clear that the set of unpaired states is convex. This suggests the use of the Hahn-Banach separation theorem as a means to certify that a given density operator is not in the set of paired states. In analogy to the entanglement witnesses in quantum-information theory [39], we define the following:

*Definition III.6*. A *pairing witness* $W$ is a Hermitian operator that fulfills $\mathrm{tr}[W\rho_u] \geq 0$ for all unpaired states $\rho_u$, and for which there exists a paired state $\rho$ such that $\mathrm{tr}[W\rho] < 0$. We then say that *W detects* the paired state $\rho$.

The witness defines a hyperplane in the space of density operators such that the convex set of unpaired states lies wholly on that side of the plane characterized by $\mathrm{tr}[\rho W] > 0$. According to the Hahn-Banach theorem [40], for every unpaired state there exists a witness operator that detects it. In principle, a witness operator can be an operator involving an arbitrary number of creation and annihilation operators. However, since definition of pairing refers only to expectation values of operators in $A_2$, it is enough to restrict to

[2] Note that our basis-independent definition clearly has no relation to entanglement of modes, which is basis-dependent. The product states of Def. II.1 can be mode-entangled for some choice of partition of modes, e.g., $(1/\sqrt{2})(a_1^\dagger + a_2^\dagger)|0\rangle$ is entangled in modes $a_1^\dagger$ and $a_2^\dagger$.

operators from that set. This represents a significant simplification both mathematically (witness operators from a finite dimensional set) and experimentally, since operators involving more than two-body correlations are typically very difficult to measure.

The construction of entanglement witnesses detecting all entangled states is an unsolved problem in entanglement theory, and we will not be able to give a complete solution to the problem of finding all pairing witnesses either. However, in Sec. V we will construct witnesses for a large subclass of BCS states by using the correspondence between number-conserving and Gaussian BCS states.

Whether a state $\rho$ is paired can be determined from a finite set of real numbers, namely the expectation values of a Hermitian basis $\{O_\alpha\}$ of $A_2$. This allows us to reformulate the pairing problem as a geometric question on convex sets in finite-dimensional Euclidean space, describe a complete set of pairing witnesses, and deduce a relation to the ground-state energies of quadratic Hamiltonians.

Consider a set $\{O_\alpha, \alpha=1,\ldots,K\}\subset A_2$ of Hermitian operators in $A_2$ that are not necessarily a basis. Denote by $\vec{O}$ the vector with components $O_\alpha$. We define the set of all expectation values of $\vec{O}$ for separable states

$$C_{\vec{O}} = \{\vec{v} = \mathrm{tr}[\vec{O}\rho_s]: \rho_s \in S_{\mathrm{sep}}\} \subset \mathbb{R}^K. \tag{20}$$

For a state $\rho$, let $\vec{v}_\rho \equiv \mathrm{tr}[\vec{O}\rho]$. By definition, $\rho$ is paired if $\vec{v}_\rho \notin C_{\vec{O}}$. As the set of separable states is convex, so is $C_{\vec{O}}$. Hence, we can use a result of convex analysis to check if $\vec{v}_\rho \notin C_{\vec{O}}$ (see, e.g., [41]):

*Lemma III.7.* Let $C\subset\mathbb{R}^N$ be a closed convex set, and let $\vec{v}\in\mathbb{R}^N$. Then

$$\vec{v} \in C \Leftrightarrow \forall\, \vec{r} \in \mathbb{R}^N: \vec{v}\cdot\vec{r} \geq E(\vec{r}) = \inf_{\vec{w}\in C} \vec{w}\cdot\vec{r}. \tag{21}$$

For our purposes, this translates into the following result:

*Lemma III.8.* For a vector of observables $\vec{O}=(O_1,\ldots,O_K)$ let $H(\vec{r})=\vec{r}\cdot\vec{O}$ and $E(\vec{r})=\inf_{\rho\in\mathcal{S}_{\mathrm{sep}}}\{\mathrm{tr}[H(\vec{r})\rho]\}$. Then $W(\vec{r})\equiv H(\vec{r})-E(\vec{r})$ is a pairing witness, whenever $E(\vec{r})\neq\inf_{\mathrm{all}\ \rho}\{\mathrm{tr}[\rho H(\vec{r})]\}$.

If $\{O_\alpha\}$ form a basis of $A_2$, then $W(\vec{r})$ is a complete set of witnesses in the sense that all paired states are detected by some $W(\vec{r})$, i.e., $\rho$ is unpaired iff $\mathrm{tr}[W(\vec{r})\rho]\geq 0 \forall\ \vec{r}$.

*Proof.* The witness property of $W(\vec{r})$ is obvious from the definition of $E(\vec{r})$.

For the second part, "if" is clear and "only if" is seen as follows: By Lemma III.7, if $\mathrm{tr}[W(\vec{r})\rho]\geq 0\forall\ \vec{r}$, then $\vec{v}_\rho\in C$, i.e., the expectation values can be reproduced by a separable state. But since all expectation values of operators $\in A_2$ can be computed from $\vec{v}_\rho$, this implies all two-particle expectations of $\rho$ can be thus reproduced, i.e., $\rho$ is unpaired. □

For an $M$-mode system with annihilation operators $a_i$, a standard choice of $O_\alpha$ is, e.g., given by the real and imaginary parts of $\{(a_i^\dagger a_j^\dagger a_k a_l)_{i>j,k>l},(a_i^\dagger a_j^\dagger)_{i>j},(a_i^\dagger a_j)_{i\geq j}\}$, i.e., the dimension of $A_2$ (as a real vector space) is $K=M^2(M-1)^2/2+2M^2$.

Thus Lemma III.8 gives a necessary and sufficient criterion of pairing and provides a geometrical picture of the pairing problem. While the proof that a state is unpaired will in general be difficult as it requires knowledge of all $E(\vec{r})$ and experimentally the measurement of a complete set of observables, practical sufficient conditions for pairing can be obtained by restricting to a subset $O\subset A_2$. We will show in Sec. V A that for a certain choice of $\{O_\alpha\}\subset A_2$, the set $C_{\vec{O}}$ has a very simple form and allows a good visualization of the geometry of paired states and the detection of all BCS states up to passive transformations.

To provide a way to determite $E(\vec{r})$ used in Lemma III.8, we point out an interesting connection to the covariance matrices $\Gamma_c$ [cf. Eq. (11)] of Gaussian states: even for number-conserving states, $E(\vec{r})$ is given by a quadratic minimization problem in terms of $\Gamma_c$.

*Lemma III.9.* Let $E(\vec{r})$ and $H(\vec{r})$ be as in Lemma III.8 and let $\vec{O}=\{a^\dagger{}_i a^\dagger{}_j a_k a_l, a^\dagger{}_i a_j\}$ and group the components of $\vec{r}$ in two subsets $(\vec{r})_{ijkl}$ and $(\vec{r})_{ij}$ corresponding to the one- and two-particle observables, respectively. Then $E(\vec{r})$ is given by a quadratic minimization problem over complex covariance matrices Eq. (11), in particular the off-diagonal block $R$ of $\Gamma_c$. We have

$$E(\vec{r}) = \inf_{\substack{R=-R^\dagger\\ 4R^2=-\mathbb{1}}} \{\vec{\gamma}^T M(\vec{r})\vec{\gamma} + w(\vec{r})^T\vec{\gamma}\}, \tag{22}$$

where $(\vec{\gamma})_{kl}=\langle a^\dagger{}_k a_l\rangle = -iR_{lk}+\frac{1}{2}\delta_{kl}$ and the $\vec{r}$-dependent quantities are $[M(\vec{r})]_{(ik)(jl)}=-\vec{r}_{ijkl}+\vec{r}_{ijlk}$ and $[w(\vec{r})]_{kl}=\vec{r}_{kl}$. The minimization can be extended over *all* (not necessarily pure separable) CMs without changing the result.

*Proof.* The minimum $\min_{\rho\in\mathcal{S}_{\mathrm{sep}}}\{\langle H(\vec{r})\rangle_\rho\}$ is attained for *pure* separable states, i.e., product states. All pure fermionic product states are Gaussian; then by Wick's theorem, the expectation values of the $O_{ijkl}=a^\dagger{}_i a^\dagger{}_j a_k a_l$ factorize as $\langle a^\dagger{}_i a^\dagger{}_j a_k a_l\rangle_\rho = \langle a^\dagger{}_i a^\dagger{}_j\rangle\langle a_k a_l\rangle - \langle a^\dagger{}_i a_k\rangle\langle a^\dagger{}_j a_k\rangle + \langle a^\dagger{}_i a_l\rangle\langle a^\dagger{}_j a_k\rangle$. Since product states are also number-conserving, the first term vanishes. For the other two we use that $\langle a^\dagger{}_k a_l\rangle = -iR_{lk}+\frac{1}{2}\delta_{kl}$, i.e., they only depend on the off-diagonal block $R$. The pure state condition $\Gamma^2=-\mathbb{1}$ translates into $4R^2=-\mathbb{1}$ for product states $Q=0$.

We could extend over all CMs $\gamma_c$ since only the block $R$ appears in the expression to be minimized over, and since if $\Gamma_c(Q,R)$ is a valid CM, then so is $\Gamma_c(0,R)$. ■

This lemma provides a systematic way to construct pairing witnesses.

### D. Pairing measures

It would be desirable if a theory of pairing not only answers the question of whether a state is paired, but also quantifies the amount of pairing inherent in a state. For this purpose, we introduce the notion of a pairing measure:

*Definition III.10.* Let $\rho$ be an $M$-mode fermionic state. A pairing measure is a map

$$\mathcal{M}: \rho \mapsto \mathcal{M}(\rho) \in \mathbb{R}_+,$$

which is invariant under passive transformations and fulfills $\mathcal{M}(\rho)=0$ for every unpaired state $\rho$.

In addition, it is often useful to normalize $\mathcal{M}$ such that $\mathcal{M}(\rho_0)=1$ defines the "unit of pairing." The pair state $|\Phi\rangle$ of Eq. (19) would be an obvious choice for this unit, but as we see in Sec. IV D for Gaussian states a different unit is more natural, therefore we do not include normalization in the above definition.

In the geometric picture of the previous section, a candidate for a pairing measure that immediately comes to mind is the distance of $\vec{v}_\rho$ from the set $C$. This measure is positive, and it is invariant under passive transformations, as those correspond to a basis change in the space of expectation vectors.

The computation of this distance is, in general, very difficult and there is no evident operational meaning to this quantity. In the following sections, we will introduce a different measure that can be computed for relevant families of states and allow a physical interpretation in terms of quantifying a resource for precision measurements.

## IV. PAIRING FOR GAUSSIAN STATES

In this section, we study pairing of fermionic Gaussian states. We start with the construction of pairing witnesses in Sec. IV A, which will later be a useful guideline for the construction of pairing witnesses for number-conserving states. Then we derive a simple necessary and sufficient criterion for pairing of Gaussian states. In Sec. IV C, we show how pure fermionic Gaussian states can be connected to an SU(2) angular momentum representation. This picture will guide us to the construction of a pairing measure.

### A. Pairing witnesses for Gaussian states

Pairing witnesses for pure Gaussian states emerge naturally from the property that every such state is the ground state of a quadratic Hamiltonian (see Sec. II C). This leads to the following theorem:

*Theorem IV.1.* Let $0<\epsilon<1$ and let $0\leqslant|v_k|^2\leqslant 1-\epsilon$ and $\Sigma_k|v_k|^2>0$. Then the operator

$$H=\sum_{k=1}^{M}2(1-\epsilon-|v_k|^2)(n_k+n_{-k})-2v_ku_k^*P_k^\dagger-2v_k^*u_kP_k \tag{23}$$

is a pairing witness, detecting

$$|\Psi_{\mathrm{Gauss}}\rangle=\prod_k(u_k+v_kP_k^\dagger)|0\rangle.$$

*Proof.* Every Gaussian state is the ground state of a quadratic Hamiltonian. In particular, $|\Psi_{\mathrm{Gauss}}\rangle$ is seen to be the ground state of

$$H_0=\sum_{k=1}^{M}(|u_k|^2-|v_k|^2)(n_k+n_{-k}-1)-2v_ku_k^*P_k^\dagger-2v_k^*u_kP_k$$

with the help of Eqs. (13) and (14), as the Hamiltonian matrix of $H_0$ and $\Gamma$ can be brought simultaneously to the standard forms (5) and (7), respectively. Subtracting the minimal energy for separable states,

$$E_{\min}^{\mathrm{sep}}=-(1-2\epsilon)\Sigma_k\langle n_k+n_{-k}\rangle-(|u_k|^2-|v_k|^2)$$

(note that $\langle P_k\rangle=0$ for separable states), we arrive at the Hamiltonian (23). For separable states $\rho$, the expectation values of $P_k^\dagger$ vanish, so that $\mathrm{tr}[H\rho]\geqslant 0$. For the Gaussian BCS state, however, $\langle\Psi_{\mathrm{Gauss}}|H|\Psi_{\mathrm{Gauss}}\rangle=-4\epsilon\Sigma_k|v_k|^2<0$. ■

### B. Complete solution of the pairing problem for fermionic Gaussian states

Every Gaussian state is completely characterized by its covariance matrix, so that the solution of the pairing problem must be related to it. The pairing problem is completely solved by the following theorem:

*Theorem IV.2.* Let $\rho$ be the density operator of a fermionic Gaussian state with covariance matrix $\Gamma_c$ defined in Eq. (11). Then $\rho$ is paired iff $Q\neq 0$.

*Proof.* First, note that the condition $Q=0$ is independent of the choice of basis. If $\rho$ is not paired, then there exists a separable state having the same covariance matrix as $\rho$. This implies $Q=0$, as separable states are convex combinations of states with fixed particle number, and thus $\langle i/2[a_k,a_l]\rangle=0$.

Now, let $\Gamma_c$ be the covariance matrix of a paired Gaussian state, and assume that $Q=0$. As $R$ is anti-Hermitian, there exists a passive transformation such that $R_{ij}=r_i\delta_{ij}$, and $Q=0$ is unchanged. But such a covariance matrix can be realized by a separable state fulfilling $\langle n_i\rangle=r_i$ in contradiction to the assumption.

Note that Thm. IV.2 implies that a Gaussian state is unpaired iff it is number-conserving.

### C. Angular momentum algebra for Gaussian states

In this section, we will show that pairing of Gaussian states can be understood in terms of an SU(2) angular momentum algebra. The expectation values of the angular momentum operators can be visualized using a Bloch sphere, giving us further understanding of the structure of pairing in Gaussian states. It later leads to the construction of a pairing measure for these states. Define the operators [42,43]

$$j_k^{(x)}=\frac{1}{2}(P_k^\dagger+P_k),$$

$$j_k^{(y)}=\frac{i}{2}(P_k^\dagger-P_k),$$

$$j_k^{(z)}=\frac{1}{2}(1-n_k-n_{-k}).$$

They fulfill $[j_k^{(a)},j_k^{(b)}]=i\varepsilon_{abc}j_k^{(c)}$, $a,b,c\in\{x,y,z\}$, forming an SU(2) angular momentum algebra. For pure Gaussian states in the standard form (15), the expectation values of the angular momentum operators are given by $\langle j_k^{(x)}\rangle=\mathrm{Re}(u_kv_k^*)$, $\langle j_k^{(y)}\rangle=\mathrm{Im}(u_kv_k^*)$, and $\langle j_k^{(z)}\rangle=\frac{1}{2}(1-2|v_k|^2)$. As $j^2=\Sigma_{i=x,y,z}\langle j_k^{(i)}\rangle^2=\frac{1}{4}$ independent of $u_k$ and $v_k$, the expectation values for every pure Gaussian state lie on the surface of a sphere with radius $\frac{1}{2}$. As we have shown in Thm. 4.2, every unpaired state $\rho_u$ fulfills $\langle j_k^{(x)}\rangle_{\rho_u}=\langle j_k^{(y)}\rangle_{\rho_u}=0$, so that these states are

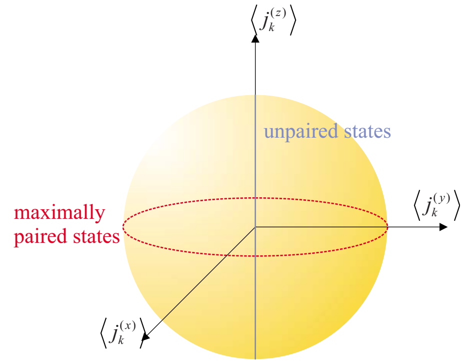


FIG. 1. (Color online) Bloch sphere representation of the expectation values of $j_k^{(x)}$, $j_k^{(y)}$, and $j_k^{(z)}$ for a variational BCS state. All pure states lie on the surface of the sphere. Unpaired states lie on the $z$ axis, while the maximally paired states lie on the equator.

located on the $z$ axis. The states on the equator have $\langle j_k^{(x)}\rangle^2 + \langle j_k^{(y)}\rangle^2 = \frac{1}{4}$, i.e. they correspond to $|u_k|^2 = |v_k|^2 = \frac{1}{2}$. The situation is depicted in Fig. 1. Referring to the states on the equator as maximally paired is suggested by the fact that they have maximal distance from the set of separable states. This intuitive picture is further borne out by two observations: first, the states on the equator display maximal entanglement between the involved modes [30]. Second, they have the property[3] that they achieve the minimal expectation value of any quadratic witness operator (up to basis change). To see this, recall from Sec. II C that any quadratic Hamiltonian of two modes $k,-k$ is (up to a common factor and basis change) of the form $\alpha\mathbb{1} + \sin\theta(n_k + n_{-k}) + \cos\theta(P_k^\dagger + P_k)$. It is a witness (i.e., has positive expectation for all product states) if $\alpha \geq |\max\{0, 2\sin\theta\}|$ and does detect some paired state as long as $\sin\theta > -1$. The minimum eigenvalue is $\sin\theta - 1 + \alpha$ and the minimum $\mathrm{tr}(W\rho) = -1$ is attained for $\rho = \frac{1}{2}(1 + P_k^\dagger)|0\rangle\langle 0|(1 + P_k)$.

The pairing measure, which is the topic of the next section, will confirm the characterization as maximally paired.

### D. A pairing measure for Gaussian states

The angular momentum representation of paired states depicted in Fig. 1 suggests the introduction of a pairing measure via a quantity related to $|\langle j_k^{(x)}\rangle_{\rho_G}|^2 + |\langle j_k^{(y)}\rangle_{\rho_G}|^2 = |\langle a^\dagger{}_k a^\dagger{}_{-k}\rangle_{\rho_G}|^2$:

*Definition IV.3*. Let $\rho$ be a fermionic state, and let $Q_{kl} = i/2\,\mathrm{tr}(\rho[a_k, a_l])$. Then we define

$$\mathcal{M}_G(\rho) = 2\|Q\|_2^2 = 2\sum_{kl} |Q_{kl}|^2. \quad (24)$$

*Lemma IV.4*. $\mathcal{M}_G$ as defined in Def. IV.3 is a pairing measure fulfilling $\mathcal{M}_G(\rho) \leq M$ for every $M$-mode Gaussian state.

*Proof*. Under a passive transformation $Q \mapsto UQU^T$, and hence $\|Q\|_2^2$ is invariant. Further, we know by Thm. 4.2 that $Q=0$ for unpaired states.

[3] Maximally entangled states of two qubits share an analogous property about entanglement witnesses [44].

It remains to show that for an $M$-mode Gaussian state $\rho$ we have $\mathcal{M}_G(\rho) \leq M$. Let $\Gamma_c$ be the $2M \times 2M$ covariance matrix of $\rho$ defined in Eq. (11). We show first that $\mathcal{M}(\rho)$ is maximized for pure Gaussian states. To do so, recall that an admissible covariance matrix for a Gaussian state in the real representation has to fulfill $i\Gamma \leq 1$ with equality iff $\Gamma$ is the covariance matrix of a pure Gaussian state. This translates into $\Gamma_c\Gamma_c^\dagger \leq \mathbb{1}$ with equality iff $\Gamma_c$ belongs to a pure Gaussian state. Using the form of $\Gamma_c$ given in Eq. (11), this implies $2\,\mathrm{tr}[QQ^\dagger + RR^\dagger] \leq \mathrm{tr}[\mathbb{1}] = 2M$. Hence, $\|Q\|_2^2 \leq M - \|R\|_2^2$. It follows that for a fixed value of $\|R\|_2^2$, the value of $\|Q\|_2^2$ is maximal for a pure Gaussian state. Further, the standard form (15) implies that for every value of $\|R\|$ such a state exists, and that the maximal value is given by $\|Q\|_2^2 = 2\sum_{k=1}^M |u_k|^2|v_k|^2 \leq M/2$, as $|u_k|^2 + |v_k|^2 = 1$. ■

Hence, for every pure Gaussian state with standard form (15) the value of the pairing measure is given by $\mathcal{M}_G(\rho) = 4\sum_{k=1}^M |u_k|^2|v_k|^2$. Since $|v_k|^2 = 1 - |u_k|^2$, the measure attains its maximum value for $|u_k|^2 = |v_k|^2 = 1/2$, i.e., for the states already identified as maximally paired.

$\mathcal{M}_G(\rho)$ will appear again when we study the use of paired states for metrology applications, linking the pairing measure to the usefulness of a state for quantum phase estimation and giving support to the "resource" character of paired states.

## V. PAIRING OF NUMBER-CONSERVING STATES

In the preceding section, we gave a complete solution to the pairing problem for fermionic Gaussian states. There, Wick's theorem lead to a reduction of the problem to properties of the covariance matrix. For number-conserving systems, the situation is more complicated, as now also operators of the form $a_i^\dagger a_j^\dagger a_k a_l$ have to be taken into account. However, we will derive pairing witnesses capable of detecting all number-conserving BCS states in Sec. V A using the concept of convex sets. For certain classes of BCS states, we will construct a family of improved witnesses using the analogy to the Gaussian states. Witnesses have the drawback that they depend on the choice of basis. That is, even if a witness detects $\rho$, it does not detect all states related to $\rho$ by a passive transformation. We will show that the eigenvalues of the reduced two-particle density matrix can be used to obtain a sufficient criterion for pairing in Sec. V B that is basis-independent. We close the section with the construction of a pairing measure in Sec. V C.

### A. Pairing of all BCS states and geometry of paired states

In a realistic physical setup, it may not be practical to perform all the measurements needed according to Lemma III.8 to check the necessary and sufficient condition for pairing. Having access only to a restricted set of measurements, necessary criteria for pairing can be derived. In this section, we consider the simplest case of a symmetric measurement involving four modes, i.e., we are looking at the following vector of operators:

$$\vec{O}_3 = \begin{pmatrix} n_k + n_{-k} + n_l + n_{-l} \\ n_k n_{-k} + n_l n_{-l} \\ a_k^\dagger a_{-k}^\dagger a_{-l} a_l + \mathrm{H.c.} \end{pmatrix}. \quad (25)$$

Remarkably, these expectation values will turn out to be sufficient to detect all BCS states as paired.

We are interested in $C_{\vec{O}_3}^{\text{unpaired}}=\{\text{tr}(\vec{O}_3\rho):\rho \text{ separable}\}$, the set of all expectation values of $\vec{O}_3$ that correspond to separable states. If for some $\rho$ the vector $\vec{v}_\rho=\text{tr}(\vec{O}_3\rho)$ is found outside of $C_{\vec{O}_3}^{\text{unpaired}}$, then it follows from Lemma III.8 that $\rho$ is paired. Membership in $C_{\vec{O}_3}^{\text{unpaired}}$ can be easily checked by the following Lemma:

*Lemma V.1*. A number-conserving state $\rho$ has expectation values of $\vec{O}_3$ [see Eq. (25)] compatible with separability if and only if $\text{tr}(H_{k\pm}^{(p)}\rho)\geqslant 0$ for $k=1,2,3$, where

$$H_{1\pm}^{(p)}=\frac{1}{2}(n_k+n_{-k}+n_l+n_{-l})-(n_kn_{-k}+n_ln_{-l}) \pm (a_k^\dagger a_{-k}^\dagger a_{-l}a_l+\text{H.c.}), \quad (26)$$

$$H_{2\pm}^{(p)}=(n_kn_{-k}+n_ln_{-l})\pm(a_k^\dagger a_{-k}^\dagger a_{-l}a_l+\text{H.c.}), \quad (27)$$

$$H_{3\pm}^{(p)}=1-\frac{1}{2}(n_k+n_{-k}+n_l+n_{-l})+\frac{1}{2}(n_kn_{-k}+n_ln_{-l}) \pm\frac{1}{2}(a_k^\dagger a_{-k}^\dagger a_{-l}a_l+\text{H.c.}). \quad (28)$$

Hence, the extremal points of the set $C_{\vec{O}_3}^{\text{unpaired}}$ are given by $\text{tr}(H_{k\pm}^{(p)}\rho)=0$ for three of the witnesses (26)–(28). The faces of $C_{\vec{O}_3}^{\text{unpaired}}$ consist of points for which at least one of the expectation values $\text{tr}(H_{k\pm}^{(p)}\rho)$ vanishes. $H_{1\pm}^{(p)}$ and $H_{3\pm}^{(p)}$ are also pairing witnesses, while $H_{2\pm}^{(p)}$ is nonnegative on all number-conserving states.

*Lemma V.2*. Every number-conserving fermionic state fulfills $\text{tr}(H_{k\pm}\rho)\geqslant 0$, where

$$H_1=\frac{1}{2}(n_k+n_{-k}+n_l+n_{-l})-(n_kn_{-k}+n_ln_{-l}), \quad (29)$$

$$H_{2\pm}=(n_kn_{-k}+n_ln_{-l})\pm(a_k^\dagger a_{-k}^\dagger a_{-l}a_l+\text{H.c.}), \quad (30)$$

$$H_{3\pm}=2-\frac{1}{2}(n_k+n_{-k}+n_l+n_{-l})\pm(a_k^\dagger a_{-k}^\dagger a_{-l}a_l+\text{H.c.}). \quad (31)$$

The extremal points of the set $C_{\vec{O}_3}^{\text{all}}=\{\text{tr}(\vec{O}_3\rho):\rho \in \mathcal{S}(\mathcal{A}_M^{(N)}):M,N\in N\}$ are given by $\text{tr}(H_{k\pm}\rho)=0$ for three of the witnesses (29)–(31). The faces of $C_{\vec{O}_3}^{\text{all}}$ consist of points for which at least one of the expectation values $\text{tr}(H_{k\pm}\rho)$ vanishes.

The proofs of the two lemmas can be found in Appendix B. We denote by $C^{\text{unpaired}}$ and $C^{\text{all}}$ the polytopes containing all expectation vectors $\vec{v}_\rho$ corresponding to unpaired states or all number-conserving states, respectively. They are bounded by six and five planes, respectively, defined through the witnesses given in Lemmas V.1 and V.2. The situation is depicted in Fig. 2.

The witnesses $H_{1\pm}^{(p)}$ given in Eqs. (26) allow us to detect all number-conserving BCS states as paired:

*Lemma V.3*. The number-conserving BCS state $|\Psi_{\text{BCS}}^{(N)}\rangle$ given in Eq. (17) is (except for the trivially unpaired cases $\alpha_k=\delta_{kk_0}$ and $N=M$) detected by the witness $H_p^{(1)}$ by choosing any two modes $(k,l)$.

*Proof*. The first two terms in $H_{1\pm}^{(p)}$ are designed such that their expectation value vanishes for states such as $|\Psi_{\text{BCS}}^{(N)}\rangle$: Since we either have a pair or no particles in the modes $(k,-k)$, we are in an eigenstate with eigenvalue 0 of the operators $n_k+n_{-k}-2n_kn_{-k}$.

The expectation value of the third term is found using the representation Eq. (18) as $|C_N|^2N!^2\text{Re}(\alpha_k\alpha_l^*)\Sigma_{j_1<\cdots<j_{N-1},\, j_i\neq k,l}|\alpha_{j_1}|^2\cdots|\alpha_{j_{N-1}}|^2$, which is nonzero unless $N=M$ or all but one $\alpha_k\neq 0$. The sign can be adjusted by a passive transformation to give $\langle H_{1+}^{(p)}\rangle_{\text{BCS}}^{(N)}<0$. ■

This shows that indeed all BCS states are paired, as desired.

The witnesses $H_{p\pm}^{(1)}$, while detecting every BCS state as paired, are in general far from optimal. As the number-conserving BCS states appear in many physical setting, like in the BEC-BCS crossover [45], it is desirable to construction improved witnesses tailored for this class of states. For BCS states realized in nature, it is often appropriate to assume some symmetry of the wave function $|\Psi_{\text{BCS}}^{(N)}(\alpha_k)\rangle=(\Sigma_{k=1}^{2M}\alpha_kP_k^\dagger)^N\;|0\rangle$. For example, if $P_k^\dagger=a_{\vec{k}\uparrow}^\dagger a_{-\vec{k}\downarrow}^\dagger$, $P_{k+M}^\dagger=a_{-\vec{k}\uparrow}^\dagger a_{\vec{k}\downarrow}^\dagger$ and if we are dealing with an isotropic setting, $\alpha_k=\alpha_{k+M}$ will hold. It is further often appropriate to assume that the number of modes is much bigger than the number of particles, i.e., $M\gg N$. For this kind of state we will construct pairing witnesses via the correspondence to the Gaussian picture. We sketch the idea of this construction leading to Thm. V.4, and give the details in the Appendix C.

We have shown in Sec. II D the connection of the Gaussian wave function and the number-conserving wave function

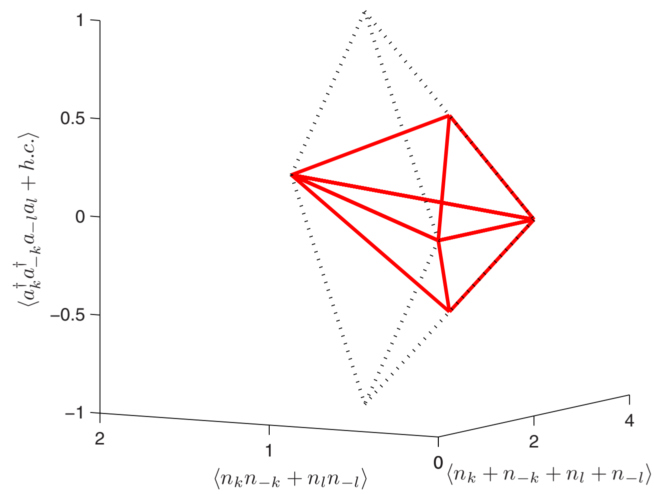


FIG. 2. (Color online) Expectation values of the vector Eq. (25). For all number-conserving states these lie within the convex set $C_{\vec{O}_3}^{\text{all}}$ indicated by the dashed back lines. The extreme points of the polytope are given by (0, 0, 0), (2, 0, 0), (4, 2, 0), and $(2,1,\pm 1)$. Unpaired states have expectation values in the smaller convex set $C_{\vec{O}_3}^{\text{unpaired}}$ (solid red), which has extreme points (0, 0, 0), (2, 0, 0), (4, 2, 0), and $(2,1/2,\pm 1/2)$.

via $|\Psi_{\text{Gauss}}\rangle = \Sigma_{k=1}^{N}\lambda_N|\Psi_{\text{BCS}}^{(N)}(\alpha_k)\rangle$. Consider a number-conserving observable $O$ and denote by $\langle O\rangle_{\text{Gauss}}$ and $\langle O\rangle_N$ its expectation value for the Gaussian and $2N$-particle BCS wave function, respectively. If the distribution of $|\lambda_N|^2$ is sharply peaked around some average particle number $\bar{N}$ with width $\Delta$, then $\langle O\rangle_{\text{Gauss}} \approx \langle O\rangle_N$ for any integer $N \in [\bar{N}-\Delta, \bar{N}+\Delta]$. In Thm. IV.1, we have constructed witnesses $H$ for all Gaussian BCS states. As these witnesses are optimal, they suggest to constitute an improved witness detecting the corresponding number-conserving BCS state. But $H$ includes terms of the form $P_k^\dagger$ that do not conserve the particle number. Hence, this witness cannot be applied directly to the number-conserving case. Using Wick's theorem, $\langle P_k^\dagger P_{k+M}\rangle_{\text{Gauss}} = \bar{u}_k v_k \langle P_k^\dagger\rangle_{\text{Gauss}}$ holds under our symmetry assumption. This suggests that we replace the non-number-conserving operator $u_k v_k P_k^\dagger$ by the number-conserving operator $P_k^\dagger P_{k+M}$. We define operators

$$H_k = 2(1-\epsilon-|v_k|^2)N_k - 4(P_k^\dagger P_{k+M} + \text{H.c.}), \tag{32}$$

$$N_k = n_k + n_{-k} + n_{k+M} + n_{-(k+M)}, \tag{33}$$

where $0 \leqslant |v_k|^2 \leqslant 1-\epsilon \forall\, k$ for $\epsilon > 0$. Further, we introduce the notation $\alpha_k = v_k/\sqrt{1-|v_k|^2}$, $\tilde{N} = \Sigma_{k=1}^{M}|v_k|^2$ and we denote by $N$ the biggest integer fulfilling $\bar{N}-\tilde{N} \geqslant 0$. Then the following holds:

*Theorem V.4.* Let $M$, $\tilde{N} \in \mathbb{N}$ and let $1 \leqslant N < 2M$. If $1 > \epsilon \geqslant 18/\sqrt{\pi\bar{N}}$, the Hamiltonian $H(\{v_k\}) = \Sigma_{k=1}^{M} H_k$ is a pairing witness detecting

$$|\Psi_{\text{BCS,sym}}^{(N)}\rangle = C_N\left(\sum_{k=1}^{M}\alpha_k(P_k^\dagger + P_{k+M}^\dagger)\right)^N|0\rangle.$$

The proof is given in Appendix C.

### B. Eigenvalues of the two-particle reduced density matrix

In this section, we derive a basis-independent condition for detecting pairing. The two-particle reduced density matrix $O$ contains all two-particle correlations. As a change of basis, $a_i^\dagger \mapsto \Sigma_k U_{ik} a_k^\dagger$ leaves the spectrum of $O$ unchanged since

$$O_{(ij),(kl)}^{(\rho)} \to (U\otimes U)_{(ij),(mn)} O_{(mn),(pq)}^{(\rho)} (U\otimes U)_{(pq),(kl)}^\dagger,$$

and we are led to the following theorem:

*Theorem V.5.* Let $\rho$ be an unpaired state, and let $O$ be its two-particle RDM $O$. Then $\lambda_{\max}(O) \leqslant 2$, where $\lambda_{\max}$ denotes the maximal eigenvalue.

*Proof.* If $\rho$ is unpaired, then there exists a separable state $\rho_s \in \mathcal{S}_{\text{sep}}$ having the same two-particle RDM. Any separable state is of the form $\rho_s = \Sigma_\alpha \mu_\alpha \rho^{(\alpha)}$, where $\rho^{(\alpha)} = |\psi^{(\alpha)}\rangle\langle\psi^{(\alpha)}|$, $|\psi^{(\alpha)}\rangle = \Pi_i a^\dagger{}_{\alpha_i}|0\rangle$, and $\Sigma_\alpha \mu_\alpha = 1$. Here, $\{a_{\alpha_i}^\dagger\}_i$ denotes some basis of mode operators. The RDM is of the form $O^{(\rho)} = \Sigma_\alpha \mu_\alpha O^{(\alpha)}$, where $O^{(\alpha)}$ is the RDM for the state $\rho^{(\alpha)}$. The RDM is calculated in the basis $\{a_i^\dagger\}_i$, and the different bases are related by a unitary transformation $a_i^\dagger = \Sigma_j U_{ik}^{(\alpha)} a_{\alpha_k}^\dagger$, so that $O_{(ij)(kl)}^{(\alpha)} = \text{tr}[\rho^{(\alpha)} a_i^\dagger a_j^\dagger a_l a_k] = (U^{(\alpha)}\otimes U^{(\alpha)})_{(ij)(mn)} O_{(mn),(pq)}^{(\alpha,0)} (U^{(\alpha)} \otimes U^{(\alpha)})_{(pq)(kl)}^\dagger$, where $O_{(mn),(pq)}^{(\alpha,0)} = \langle a_{\alpha_m}^\dagger a_{\alpha_n}^\dagger a_{\alpha_q} a_{\alpha_p}\rangle_{\rho^{(\alpha)}}$. In the basis of the $\{a_{\alpha_i}^\dagger\}_i$, the expectation value $\langle a_{\alpha_m}^\dagger a_{\alpha_n}^\dagger a_{\alpha_q} a_{\alpha_p}\rangle_{\rho^{(\alpha)}}$ is of the simple form $\langle a_{\alpha_i}^\dagger a_{\alpha_j}^\dagger a_{\alpha_l} a_{\alpha_k}\rangle_{\rho^{(\alpha)}} = \delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}$. Hence, the spectrum of the $O^{(\alpha)}$ is given by $\text{spec}(O^{(\alpha)}) = \{0,2\} \forall\, \alpha$. The two-particle RDM is Hermitian as $O_{(ij)(kl)}^\dagger = \bar{O}_{(kl)(ij)} = \langle a_k^\dagger a_l^\dagger a_j a_i\rangle = \langle a_i^\dagger a_j^\dagger a_l a_k\rangle = O_{(ij)(kl)}$. Then Weyl's theorem [46] implies $\lambda_{\max}(\Sigma_\alpha \mu_\alpha O^\alpha) \leqslant \Sigma_\alpha \mu_\alpha \lambda_{\max}(O^\alpha) \leqslant \Sigma_\alpha 2\mu_\alpha \leqslant 2$. ■

An example of a state detected as paired via criterion is the BCS state (17) with $N=2$, $M=3$, and all $\alpha_k$ equal. The largest eigenvalue of its two-particle RDM is given by $\lambda_{\max} = 8/3$.

### C. A pairing measure for number-conserving states

In Sec. IV D, we have derived a pairing measure for Gaussian states. The correspondence with number-conserving BCS states will be a guideline to derive a measure for number-conserving states. However, the measure of Def. IV.3 involves expectation values of the form $\langle a_k^\dagger a_{-k}^\dagger\rangle$ that vanish for states with fixed particle number. Yet, Wick's theorem suggests that a quantity involving expectation values of the form $\langle P_k^\dagger P_l\rangle$ will lead to a pairing measure. This is indeed the case, which is the content of the following theorem:

*Theorem V.6.* Let $\rho$ be a number-conserving pure fermionic state. Then the following quantity defines a pairing measure:

$$\mathcal{M}(\rho) = \max\left\{\max_{\{a_i^\dagger\}_i} \sum_{kl=1}^{M} |\langle P_k^\dagger P_l\rangle_\rho| - \frac{1}{2}\sum_k \langle n_k\rangle_\rho, 0\right\}, \tag{34}$$

where $P_k^\dagger = a_k^\dagger a_{-k}^\dagger$ and the maximum is taken over all possible bases of modes $\{a_i^\dagger\}_i$. For mixed states $\rho$, a measure can be defined via

$$\mathcal{M}(\rho) = \min \sum_i p_i \mathcal{M}(\rho_i), \tag{35}$$

where the minimum is taken over all possible decompositions of $\rho = \Sigma_i p_i \rho_i$ into pure states $\rho_i$.

*Proof.* The positivity of $\mathcal{M}$ and its invariance under passive transformations follow directly from the definition. It remains to show that $\mathcal{M}$ is zero for separable states. We will prove in Lemma D.1, Appendix D, that any separable state of $2N$ particles fulfills $\Sigma_{kl}|\langle P_k^\dagger P_l\rangle| \leqslant N$, and that this bound can always be achieved, which concludes the proof. ■

We close the section by calculating the value of the pairing measure for two easy examples. Let

$$|\Psi_s\rangle = \bigotimes_{k=1}^{N} \frac{1}{\sqrt{2}}(P_k^\dagger + P_{-k}^\dagger)|0\rangle, \tag{36}$$

$$|\Psi_{\text{BCS}}^{(N,M)}\rangle = C_N\left(\sum_{k=1}^{M} P_k^\dagger\right)^N|0\rangle, \tag{37}$$

the tensor product of $N$ spin-singlet states and the BCS state with equal weights, respectively. These states have a pairing measure $\mathcal{M}(|\Psi_s\rangle) = N$ and $\mathcal{M}(|\Psi_{\text{BCS}}^{(N,M)}\rangle = N(M-N)$, respectively. Thus, for the spin singlet the pairing measure has in addition the property that it is normalized to 1 and additive, while it is subadditive for $|\Psi_{\mathrm{BCS}}^{(N,M)}\rangle$. Further, this example suggests that the pairing of $\mathcal{M}(|\Psi_{\mathrm{BCS}}^{(N,M)}\rangle = N(M-N)$ is stronger than for $|\Psi_s\rangle$. We will see indeed in Sec. VI B that states of the form $|\Psi_e\rangle$ allow interferometry at the Heisenberg limit.

## VI. INTERFEROMETRY

The goal of quantum phase estimation is to determine an unknown parameter $\varphi$ of a Hamiltonian $H_\varphi = \varphi H$ at the highest possible accuracy. The value of $\varphi$ is inferred by measuring an observable $O$ on a known input state that has evolved under $H_\varphi$. In a region where the expectation value $\langle O(\varphi)\rangle$ is bijective, $\varphi$ can be inferred by inverting $\langle O(\varphi)\rangle$. In a realistic setup, however, $\langle O(\varphi)\rangle$ cannot be determined, as this would require an infinite number of measurements. Instead, one uses the mean value of the measurement results, $o$, as an estimate of $\langle O(\varphi)\rangle$. This will result in an error $\delta\varphi$ for the parameter to be estimated, as for a given value of $\varphi$ we have $\langle O(\varphi)\rangle = o \pm \sqrt{\mathrm{Var}(o)}$. Linearizing around the real value of $\varphi$, it follows that the uncertainty of $\varphi$ is given by [47,48]

$$\langle(\delta\varphi)^2\rangle = \frac{\mathrm{var}(O)}{|\partial\langle O\rangle/\partial\varphi|^2}, \tag{38}$$

where $\mathrm{var}(O) = \langle O^2\rangle - \langle O\rangle^2$, and we have used the fact that $\mathrm{var}(O) = \mathrm{var}(o)$. Further, it can be shown that the minimal uncertainty of $\varphi$ is bounded by [49,50]

$$\langle(\delta\varphi)^2\rangle \mathrm{var}(H) \geqslant \frac{1}{4\nu}, \tag{39}$$

where $\nu$ is the number of times the estimation is repeated. Equation (39) derives from the Cramér-Rao bound and is asymptotically achievable in the limit of large $\nu$.

For a given measurement scheme, i.e., for a given input state and a given observable $O$, the uncertainty in $\varphi$ can be reduced by using $N$ identical input states and average over the $N$ measurement outcomes. As the preparation of a quantum state is costly, a precision gain that has a strong dependence on $N$ is highly desirable. If these probe states are independent of each other, the precision scales like $1/\sqrt{N}$. This is the so-called standard quantum limit (SQL). Using distinguishable or bosonic systems, this limit can be beaten by a factor of $\sqrt{N}$ by using number-squeezed input states [51–54], $N$-particle path-entangled states $(\langle N,0| + \langle 0,N|)$ (NOON states), or maximally entangled GHZ states $\frac{1}{\sqrt{2}}(|N,0\rangle + |0,N\rangle)$ [48,55–57]. Achieving this so-called Heisenberg limit is the big goal of quantum metrology.

Less is known for fermionic states where number squeezing and coherent $N$-particle states are prohibited by statistics. Nevertheless, there exist fermionic $N$-particle states that can achieve the Heisenberg limit for phase measurements in a Mach-Zehnder interferometer setup [58]. Taking the existence of such states as a starting point, we show that paired fermionic states can be used as a resource for phase estimation beyond the SQL. We will consider two different settings. The first setting will be the standard Ramsey-interferometer setup of metrology, where the coupling Hamiltonian is proportional to the number operator. Here, we will see that paired states lead to a precision gain of a factor of 2 compared to separable states. The second setup involves a more complex coupling. Here it will turn out that by using paired states, the Heisenberg limit, i.e., a phase sensitivity $(\delta\varphi)^2 \sim 1/N^2$, can be achieved.

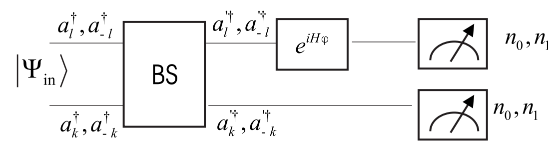


FIG. 3. Scheme of the Ramsey interferometer setup. The incoming wave function $|\Psi_{\mathrm{in}}\rangle$ enters a beam splitter (BS). Then particles in the modes $a_{\pm l}^\dagger$ evolve under the Hamiltonian $\varphi H$. At the end, a particle number measurement is performed on all particles.

### A. Ramsey interferometry with fermions

#### 1. General setup

We consider the standard Ramsey interferometer setup (see Fig. 3) where a state in the modes $\{a_{k_j}^\dagger, a_{l_j}^\dagger\}_{j=-M}^{M}$ undergoes mode mixing at a beam splitter,

$$a_{\pm k_j}^\dagger \to a_{k_j}'^\dagger = \frac{1}{\sqrt{2}}(a_{\pm k_j}^\dagger + a_{\pm l_j}^\dagger), \tag{40}$$

$$a_{\pm l_j}^\dagger \to a_{\pm l_j}'^\dagger = \frac{1}{\sqrt{2}}(a_{\pm k_j}^\dagger - a_{\pm l_j}^\dagger), \tag{41}$$

before evolving under the action of the Hamiltonian

$$H_N = \sum_{j=1}^{M} (n_{l_j} + n_{-l_j}). \tag{42}$$

Finally, a particle number measurement is performed on the system, to compute the parity

$$\mathcal{P} = (-1)^{\sum_j n_0^{(j)} + n_1^{(j)}}, \tag{43}$$

where $n_0^{(j)} = a_{k_j}'^\dagger a_{k_j}'$ and $n_1^{(j)} = a_{-k_j}'^\dagger a_{-k_j}'$. According to Eq. (38), the phase sensitivity is given by

$$(\delta\varphi)^2 = \frac{1 - \langle\mathcal{P}\rangle^2}{\left|\frac{\partial}{\partial\varphi}\langle\mathcal{P}\rangle\right|^2}, \tag{44}$$

where we have exploited $\mathcal{P}^2 = 1$. Due to the fermionic statistics, the parity operator can be written in the form

$$\mathcal{P} = \prod_{j=1}^{M} [1 - 2(n_0^{(j)} + n_1^{(j)}) + 4n_0^{(j)} n_1^{(j)}]. \tag{45}$$

In the next section, we will derive the best possible precision obtainable by using unpaired states, and compare this result to the precision achievable by using paired states. It will turn out that already at the two-particle level paired states have more power than the unpaired states for our setup.

#### *2. Bound on unpaired states for the standard interferometer*

In this section, we derive a lower bound on the phase sensitivity when using an unpaired state of $2N$ particles as input states.

*Thorem VI.1*. For the Ramsey interferometer described above, the phase sensitivity is bounded by

$$(\delta\varphi)^2 \geqslant \frac{1}{2\nu N}, \tag{46}$$

when an unpaired state of $2N$ particles is used as input state.

*Proof*. We will use Eq. (39) to derive the bound. Hence, we have to estimate an upper bound for the variance of the Hamiltonian $H_N$ defined in Eq. (42). As $H_N$ as well as $H_N^2$ contain operators from the set $A_2$ only, it is sufficient to prove the bound for product states, as for every unpaired state there exists a product state having the same expectations. In Lemma A.2 of Appendix A, we have shown that for pure separable states $\langle n_k n_l\rangle = |P_{kl}|^2 - P_{kk}P_{ll} + P_{kk}\delta_{kl}$, where $P \in \mathbb{C}^{4M\times 4M}$ is a projector of rank $2N$. We arrange the indices as $-l_M, \dots, l_M, -k_M, \dots, k_M$ and partition the projector $P$ such that $P = \left(\begin{smallmatrix} A & B \\ B^\dagger & C\end{smallmatrix}\right)$, where $A, B, C \in \mathbb{C}^{2M\times 2M}$. Then

$$\mathrm{var}(H_N) = \sum_{i=1}^{2M} A_{ii} - \sum_{i,j=1}^{2M} |A_{ij}|^2 = \mathrm{tr}[BB^\dagger], \tag{47}$$

as $H_N$ only involves the modes $-l_M, \dots, l_M$. In the last step we have used $P^2 = P$, implying $A - A^2 = BB^\dagger$. As $\mathrm{rank}(P) = 2N$, there exists some unitary $U$ such that $P = U \mathrm{Id}_{2N} U^\dagger$, where $\mathrm{Id}_{2N} = \left(\begin{smallmatrix} 1_{2N} & 0 \\ 0 & 0\end{smallmatrix}\right) \in \mathbb{C}^{4M\times 4M}$. Partitioning the unitary $U = \left(\begin{smallmatrix} U_{11} & U_{12} \\ U_{21} & U_{22}\end{smallmatrix}\right)$, where $U_{ij} \in \mathbb{C}^{2M\times 2M}$, $i,j = 1,2$, the projector $P$ is of the form

$$P = \begin{pmatrix} U_{11}\mathrm{Id}_{2N}U_{11}^\dagger & U_{11}\mathrm{Id}_{2N}U_{21}^\dagger \\ U_{21}\mathrm{Id}_{2N}U_{11}^\dagger & U_{21}\mathrm{Id}_{2N}U_{21}^\dagger \end{pmatrix}.$$

Using the above representation of $P$ and the cyclicity of the trace, we can write $\mathrm{var}(H_N) = \mathrm{tr}[\tilde{A}\tilde{B}]$ with Hermitian matrices $\tilde{A} = \mathrm{Id}_{2N}U_{11}^\dagger U_{11}\mathrm{Id}_{2N}$, $\tilde{B} = \mathrm{Id}_{2N}U_{21}^\dagger U_{21}\mathrm{Id}_{2N}$. The trace can be interpreted as a scalar product maximized for linearly dependent $\tilde{A}$ and $\tilde{B}$. Exploiting the unitarity of $U$, one sees immediately that the variance is maximized for $\tilde{A} = c/(1+c)\mathrm{Id}_{2N}$, $\tilde{B} = 1/(1+c)\mathrm{Id}_{2N}$ for some constant $c$. Hence, $\mathrm{var}(H_N) \leqslant c/(1+c)^2\, \mathrm{tr}[\mathbb{1}_{2N}] \leqslant N/2$. Inserting this into Eq. (39), we find that $(\delta\varphi)^2 \geqslant \frac{1}{2\nu N}$. ■

#### *3. Interferometry with two particles*

In this section, we will show that already a two-particle paired state can beat the bound for the phase sensitivity using unpaired states (46). Hence pairing manifests itself as useful quantum correlation already at the two-particle level. We show the following:

*Theorem VI.2*. Using the paired state

$$|\Psi_{\mathrm{in}}^{(2)}\rangle = \left(\sum_{j=1}^{M} \alpha_j a_{k_j}^\dagger a_{-k_j}^\dagger + \beta_j a_{l_j}^\dagger a_{-l_j}^\dagger\right)|0\rangle, \tag{48}$$

with normalization $\Sigma_j |\alpha_j|^2 + |\beta_j|^2 = 1$ as input state for the Ramsey interferometer, the optimal phase sensitivity is given by

$$(\delta\varphi)^2_{\min} = \frac{1}{2[1 + 2\Sigma_{j=1}^M \mathrm{Re}(\alpha_j\beta_j^*)]} \geqslant \frac{1}{4}. \tag{49}$$

*Proof*. Take $|\Psi_{\mathrm{in}}^{(2)}\rangle$ as the input state. After an application of the beam splitter transformation (40) and an evolution under the Hamiltonian (42), the measurement outcome of the parity operator is calculated to be

$$\langle\mathcal{P}\rangle = 1 - \sin^2\varphi\left(1 + 2\sum_{j=1}^{M} \mathrm{Re}(\alpha_j\beta_j^*)\right). \tag{50}$$

Using Eq. (44), we obtain Eq. (49). The bound of $\frac{1}{4}$ can be obtained for a state where $\alpha_k = \beta_k \forall\ k$. ■

Theorem VI.2 shows that there exist two-particle paired states exceeding the bound on product states (46).

#### *4. Interferometry with 2N-particle BCS states*

Generalizing the result obtained in the last section, it follows immediately that states of the form $|\Psi_{\mathrm{in}}^{(2)}\rangle^{\otimes N}$ will lead to a phase sensitivity $(\delta\varphi)^2_{\min} = 1/\{2N[1 + 2\Sigma_{j=1}^M \mathrm{Re}(\alpha_j\beta_j^*)]\}$. In this section, we will show that the same result can be achieved using BCS states.

*Theorem VI.3*. Let the paired state

$$|\Psi_{\mathrm{in}}^{(2N)}\rangle = c'\left(\sum_{j=1}^{M} \alpha_j a_{k_j}^\dagger a_{-k_j}^\dagger + \beta_j a_{l_j}^\dagger a_{-l_j}^\dagger\right)^N |0\rangle, \tag{51}$$

where we use the normalization condition $\Sigma_j |\alpha_j|^2 + |\beta_j|^2 = 1$, be the input state for the Ramsey-type interferometer defined above. Then the optimal phase sensitivity is given by

$$(\delta\varphi)^2 = \frac{1}{2\bar{N}[1 + 2\Sigma_j \mathrm{Re}(\alpha_j\beta_j^*)]}. \tag{52}$$

*Proof*. As in previous sections, we will use the correspondence to the Gaussian state,

$$|\Psi_{\mathrm{in,Gauss}}^{(2\bar{N})}\rangle = c \exp\left[\sum_{j=1}^{M} \alpha_j a_{k_j}^\dagger a_{-k_j}^\dagger + \beta_j a_{l_j}^\dagger a_{-l_j}^\dagger\right]|0\rangle,$$

where $|N - \bar{N}| \ll \bar{N}$ for the calculation. After the state has passed through the interferometer, the expectation value of the parity operator is readily computed to be $\langle\mathcal{P}\rangle_{\mathrm{Gauss}} = \Pi_j(1 - |c|^2|\alpha_j + \beta_j|^2 \sin^2\varphi)$. As only number operators are involved, $\langle\mathcal{P}\rangle_{\mathrm{Gauss}} \approx \langle\mathcal{P}\rangle_N$, where $\langle\cdots\rangle_N$ denotes the expectation value of $\mathcal{P}$ for the state $|\Psi_{\mathrm{in}}^{(2N)}\rangle$. Expanding Eq. (44) for small values of $\varphi$ and using $\bar{N} = |c|^2\Sigma_k |\alpha_k|^2 + |\beta_k|^2 = |c|^2$, one obtains Eq. (52), which has minimal value $(\delta\varphi)^2 = 1/(4N)$. This result is obtained when $\alpha_j = \beta_j \forall\ j$. ■

The above result shows that paired states result in a precision gain of up to a factor of 2 compared to the best precision obtainable for unpaired states (46).

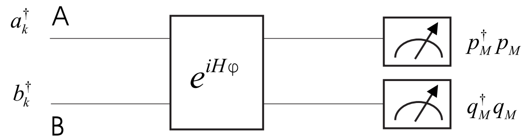


FIG. 4. Setup that allows interferometry with paired states at the Heisenberg limit. Particles in modes $a_k^\dagger$ and $b_k^\dagger$ evolve under the complex coupling Hamiltonian $H$ (for the detailed form of $H$, refer to the text). In the end, particle numbers are measured.

The pairing measure derived in Secs. IV D and V C quantifies the precision gain obtainable by the use of paired states. To see this, denote by $|\Psi^{(2\bar{N})\prime}_{\text{in,Gauss}}\rangle$ the state after the beam splitter transformation. Then the pairing measure (Def. IV.3) for this state evaluates to

$$\mathcal{M}_G(|\Psi^{(2\bar{N})\prime}_{\text{in,Gauss}}\rangle) = \frac{N^2}{2}\left(1 + 2\sum_j \text{Re}(\alpha_j\beta_j^*)\right),$$

so that

$$(\delta\varphi)^2 = \frac{\bar{N}}{4\mathcal{M}_G(|\Psi^{(2\bar{N})\prime}_{\text{in,Gauss}}\rangle}. \tag{53}$$

The above relation demonstrates that $\mathcal{M}$ is indeed quantifying a useful resource present in paired states. Whether this interpretation can be extended to mixed states will not be explored here.

### B. Interferometry involving a pair-interaction Hamiltonian

So far we have seen that paired states lead to a gain of a factor of 2 in precision compared to unpaired states in a Ramsey-type interferometer. This section will show that paired states are even more powerful and can lead to a precision gain of a factor of $N$ when measuring the phase of a pair-interaction Hamiltonian.

We consider a setup where two fermionic states enter the ports $A$ and $B$ of an interferometer. The particles entering port $A$ can occupy the modes $\{a_k^\dagger\}_{k=-M}^{M}$, while the particles entering through port $B$ can occupy the modes $\{b_k^\dagger\}_{k=-M}^{M}$. Then the two states evolve under the Hamiltonian $H_c$ to be defined below and a particle number measurement is performed at the end. The situation is depicted in Fig. 4. We will compare the power of paired states over unpaired ones for two different settings. We start by introducing some basic notation.

#### 1. Prerequisites

We define pair operators $P_k^\dagger = a_k^\dagger a_{-k}^\dagger$ and $Q_k^\dagger = b_k^\dagger b_{-k}^\dagger$ and their equally weighted superpositions

$$p_M^\dagger = \frac{1}{\sqrt{M}}\sum_{k=1}^{M} P_k^\dagger, \quad q_M^\dagger = \frac{1}{\sqrt{M}}\sum_{k=1}^{M} Q_k^\dagger. \tag{54}$$

The operators $p_M^\dagger$ and $q_M^\dagger$ fulfill the commutation relations

$$[p_M^\dagger, p_M] = -1 + \frac{1}{M}\hat{N}_a, \tag{55}$$

$$[q_M^\dagger, q_M] = -1 + \frac{1}{M}\hat{N}_b, \tag{56}$$

where $n_k = a_k^\dagger a_k$ so that $N_a = \Sigma_k(n_k + n_{-k})$, and $N_b = \Sigma_k(m_k + m_{-k})$ with $n_k = a_k^\dagger a_k$ and $m_k = b_k^\dagger b_k$ being the number operators for particles in modes $a_k^\dagger$ and $b_k^\dagger$, respectively.

We will compare the power of two paired states and two unpaired states entering through port $A$ and $B$. The bound for unpaired states will be derived again via Eq. (39). As $H_c$ and $H_c^2$ will be elements of $A_2$, it is sufficient, as in the last section, to compare the power of paired states to those of sparable states. The paired states will be of the form

$$|\Psi_N^{(M)}\rangle = |N\rangle_a^{(M)}|N\rangle_b^{(M)}, \tag{57}$$

$$|N\rangle_a^{(M)} = c_N^{(M)}(p_M^\dagger)^N|0\rangle, \quad |N\rangle_b^{(M)} = c_N^{(M)}(q_M^\dagger)^N|0\rangle, \tag{58}$$

with normalization constant $c_N^{(M)} = (NM!/M^N)^{-1/2}$, while the separable states are given by

$$|\Phi_N\rangle = |\phi^{(2N)}\rangle_a|\phi^{(2N)}\rangle_b, \tag{59}$$

where $|\phi^{(2N)}\rangle_{a,b}$ are separable states in the modes $a_k^\dagger$ and $b_k^\dagger$, respectively.

After the input state has evolved under the Hamiltonian $H_\varphi$ into the state $|\Psi_N^{(M)}(\varphi)\rangle = e^{iH_c\varphi}|\Psi_N^{(M)}\rangle$, an observable $O$ is used as an estimator to determine the parameter $\varphi$ to a precision given by Eq. (38). Instead of working in the Schrödinger picture of state evolution, it turns out to be more convenient to tackle the problem in the Heisenberg picture, where $O$ evolves according to $O \to O' = e^{-iH_c\varphi}Oe^{iH_c\varphi}$. We are interested in the phase sensitivity for small $\varphi$, so that we can expand Eq. (38) in powers of $\varphi$, arriving at

$$O(\varphi) = O - i\varphi[H_c, O] - \frac{1}{2}\varphi^2(H_c^2 O + OH_c^2 - 2H_cOH_c) + O(\varphi^3). \tag{60}$$

If the input state $|\Psi_N^{(M)}\rangle$ is an eigenvector of $O$ with eigenvalue 0, we obtain the following simple expressions for $\langle O\rangle$ and $\text{var}(O)$:

$$\left|\frac{\partial}{\partial\varphi}\langle O\rangle\right|^2 = 4\varphi^2|\langle H_cOH_c\rangle|^2 + O(\varphi^3), \tag{61}$$

$$\text{var}(O) = \varphi^2\langle H_cO^2H_c\rangle + O(\varphi^3), \tag{62}$$

so that the phase fluctuation $(\delta\varphi)^2$ simplifies to

$$(\delta\varphi)^2 = \frac{\langle HO^2H\rangle}{4|\langle HOH\rangle|^2} + O(\varphi). \tag{63}$$

An observable fulfilling this property is $O = (n_M^{(-)})^2$, where $n_M^{(-)} = \frac{1}{2}(p_M^\dagger p_M - q_M^\dagger q_M)$.

The commutation relations for $p_M^\dagger$ and $q_M^\dagger$ [Eq. (55)] imply that in the limit of infinitely many modes $M \to \infty$, the operators $p_M^\dagger$ and $q_M^\dagger$ become bosonic. We will thus start out with a scenario where the input states are in the bosonic limit and then turn our attention to a setting that is far from the bosonic limit.

#### *2. Bosonic limit*

In this section, we will consider the scenario $M \to \infty$, i.e., we are in the bosonic limit, where the limit is taken for the expectation values of the operators. We will consider a coupling of the form $H_c = \varphi H_\infty$, where

$$H_\infty = \frac{1}{2}(a_\infty^\dagger b_\infty + a_\infty b_\infty^\dagger), \tag{64}$$

and measure $(n_\infty^{(-)})^2$.

We start deriving the best precision for unpaired states using Eq. (39). We will use a finite $M$ for input state, coupling Hamiltonian, and measurement and then take the limit $M \to \infty$. To be precise, the calculation will be done for $H_M = \frac{1}{2}(a_M^\dagger b_M + a_M b_M^\dagger)$ and $(n_M^{(-)})^2$. Then $\lim_{M\to\infty}\langle \phi_{a,b}|H_M|\phi_{a,b}\rangle = 0$ due to the conservation of particle number. Hence,

$$\begin{aligned}\lim_{M\to\infty} \mathrm{var}(H_M) &= \lim_{M\to\infty}\langle H_M^2\rangle \\ &= \lim_{M\to\infty}(\langle p_M^\dagger p_M\rangle + \langle q_M^\dagger q_M\rangle)^2 = 0,\end{aligned}$$

as $\langle p_M^\dagger p_M\rangle = \frac{1}{M}\Sigma_{kl}|\langle P_k^\dagger P_l\rangle|^2 \leq N/M$, where the last inequality results from the bound of the pairing measure on unpaired states Thm. V.6. The same holds for $\langle q_M^\dagger q_M\rangle$. Hence, in the limit $M \to \infty$ the variance of $H_\infty$ vanishes. For the setting of paired states, however, we can obtain the following result:

*Theorem VI.4*. For paired input states, the interferometer depicted in Fig. 4 allows us to estimate the coupling parameter $\varphi$ to a precision

$$(\delta\varphi)_{\mathrm{inf}}^2 = \frac{1}{2N^2}. \tag{65}$$

*Proof*. Consider an interferometric setup depicted in Fig. 4, where the $2N$-particle input state and the coupling Hamiltonian are defined in Eqs. (57) and (64), respectively. We will again use a finite $M$ for input state, coupling Hamiltonian, and measurement and then take the limit $M \to \infty$, i.e., we use $|\Psi_{\mathrm{in}}\rangle = |N\rangle_a^{(M)}|N\rangle_b^{(M)}$, $H_M = \frac{1}{2}(a_M^\dagger b_M + a_M b_M^\dagger)$, and $(n_M^{(-)})^2$. Making use of the relations

$$p_M|N\rangle_a^{(M)} = \alpha_N|N-1\rangle_a^{(M)}, \tag{66}$$

$$p_M^\dagger|N\rangle_a^{(M)} = \alpha_{N+1}|N+1\rangle_a^{(M)}, \tag{67}$$

where $\alpha_N = \sqrt{N(1-(N-1)/M)}$, a lengthy but straightforward calculation leads to $(\delta\varphi)_M^2 = \frac{1}{2\alpha_{N+1}^2\alpha_N^2} + O(\varphi)$ using Eq. (63). Taking the limit $M \to \infty$ leads to the result of the theorem. ■

#### *3. Interferometry far from the bosonic limit*

In the preceding section, we have studied the power of paired states in the bosonic limit. As the power of bosonic particles for interferometry has been known for quite a while, the use of paired states where the fermionic nature of the particles survives might be a more interesting question. In this section, we will show that even far from the bosonic limit paired states can achieve a precision gain of order $N$ for quantum metrology.

We will study a coupling Hamiltonian of the form $H_c = \varphi H_F$, where

$$H_F = \sum_{k=1}^{\infty} P_k^\dagger Q_k + P_k Q_k^\dagger. \tag{68}$$

First, we will give a bound for the phase sensitivity achievable by using product states at the input:

*Theorem VI.5*. Using product states of $2N$ particles as input states for the interferometric setting depicted in Fig. 4, the phase $\varphi$ of the coupling Hamiltonian $H_c = \varphi H_F$, where $H_F$ is defined in Eq. (68), can be measured to a precision $(\delta\varphi)^2 \geq 1/(16N)$.

*Proof*. For every product state of the form (59), $\langle H_F\rangle = 0$ due to particle number conservation. Hence, $\mathrm{var}(H_F) = \langle H_F^2\rangle$. We will bound this expectation value,

$$\begin{aligned}\langle H_F^2\rangle &= \sum_{k\neq l}\langle P_k^\dagger P_l\rangle\langle Q_l^\dagger Q_k\rangle + \text{c.c.} + \sum_k \langle P_k^\dagger P_k\rangle\langle Q_k Q_k^\dagger\rangle \\ &\leq 2\Big(\sum_{k\neq l}|\langle P_k^\dagger P_l\rangle|^2\Big)^{1/2}\Big(\sum_{k\neq l}|\langle Q_k^\dagger Q_l\rangle|^2\Big)^{1/2} \\ &\quad + \sum_k \langle P_k^\dagger P_k\rangle\langle Q_k Q_k^\dagger\rangle + \text{c.c.}\end{aligned}$$

From Lemma D.1 we know that $(\Sigma_{k\neq l}|\langle P_k^\dagger P_l\rangle|^2)^{1/2} \leq \sqrt{N}$. Further, $\langle P_k P_k^\dagger\rangle = \langle 1-(\underline{n_k} - n_{-k})^2 - n_k n_{-k}\rangle \leq 1$ and $\Sigma_k\langle P_k^\dagger P_k\rangle \leq N$. Thus $\mathrm{var}(H_{pq}) \leq 2\sqrt{N}\sqrt{N} + 2N = 4N$, which leads immediately to our result via Eq. (39). ■

This bound can be beaten by a factor of $\sqrt{N}$ using paired states. A lengthy but straightforward calculation leads to the following result:

*Theorem VI.6*. Using paired states of the form (57) as input states for the interferometric setting depicted in Fig. 4, the phase $\varphi$ of the coupling Hamiltonian $H_c = \varphi H_F$, where $H_F$ is defined in Eq. (68), can be measured to a precision

$$(\delta\varphi)^2 = \frac{M(M-1)}{8N(M-N)(M-1+MN-N^2)}. \tag{69}$$

This theorem implies $(\delta\varphi)^2 \sim 1/N^2$ for all $M \geq 2N$. In conclusion, we have shown that paired states are a resource for quantum metrology. Theorem VI.6 is the main result of this section. We have remarked already at the beginning of this section that it has been proven before that the Heisenberg limit can be achieved using fermionic particles [58]. However, these states were constructed in an abstract way, while we prove that the BCS states that can be created easily in an experimental setup are a very powerful resource for quantum metrology.

## VII. APPLICATION TO EXPERIMENTS AND CONCLUSION

In summary, we have developed a pairing theory for fermionic states. We have given a precise definition of pairing based on a minimal list of natural requirements. We have seen that pairing is not equivalent to entanglement of the whole state nor of its two-particle reduced density operator but represents a different kind of quantum correlation. Within the framework of fermionic Gaussian states, we could solve the pairing problem completely. For number-conserving states, we have given sufficient conditions for the detection of pairing that can be verified by current experimental techniques, e.g., via spatial noise correlations [59–61], and we prescribed a systematic way to construct complete families of pairing witnesses.

To shed some light on the pairing debate [7,10–12], we would need access to the proportionality factor linking the quantity plotted in Fig. 4 of [7] to the local pair correlation correlation function $G_2(r,r)=\langle\Psi_\downarrow^\dagger(r)\Psi_\uparrow^\dagger(r)\Psi_\uparrow(r)\Psi_\downarrow(r)\rangle$.

Another important point of our work is the utility of fermionic states for quantum metrology. While it has been shown that, in principle, fermionic states can achieve the Heisenberg limit for precision measurements in a Ramsey-type interferometer [58], we could prove the usefulness of states that are available in the laboratory. Furthermore, the optimal precision for the Ramsey-type setup is proportional to the pairing measure introduced from an intuitive picture in Secs. II C and V. This endows the measure with an operational meaning. The results we have presented are just a first step in understanding pairing and its relation to other types of quantum correlations.

We hope that the pairing theory we have developed will help to get a better understanding of correlated many-body systems, and can provide a new perspective on quantum correlations and may serve as a starting point for further inquiries.

For example, one might attempt a finer characterization of pairing, e.g., $\Sigma_{k=1}^{2}P_k^\dagger|0\rangle$ and $\Sigma_{k=1}^{M}P_k^\dagger|0\rangle$ represent paired states of rather different nature: it would be interesting to develop witnesses or measures that allow us to determine over how many modes the pairs in a given states extend and to relate these differences to applications in metrology or elsewhere. Moreover, the theory we developed has been concerned with finitely many modes only and it is an obvious question whether generalizing to an infinite-dimensional single-particle space gives rise to new phenomena.

Up to now we have concentrated on fermionic states. But the question of pairing in bosonic systems might be equally interesting and relevant for recent experiments [62].

What about higher-order correlations? The set of unpaired states contains both separable and highly correlated states. This is, for example, reflected in the fact that there are unpaired states that can be transformed to paired ones by single-mode particle number measurements [e.g., $(a_1^\dagger a_2^\dagger a_3^\dagger + a_4^\dagger a_5^\dagger a_6^\dagger)|0\rangle$ by measuring particle number in mode $b=a_3+a_6$]. A theory of higher-order correlated states could be developed along the lines discussed here, e.g., by changing the set of observables on which the states are compared to uncorrelated ones and defining as $n$th-order correlated those states whose expectation values on $n$th-order observables cannot be reproduced by $(m<n)$-correlated states.

Tools and methods from entanglement theory have been very useful in analyzing pairing. One very important such tool, however, is missing: positive maps, that is, transformations that do not correspond to a physical operations but nevertheless, when applied to a subsystem in a separable state with the rest, map density operators to (unnormalized) density operators and thus provides strong necessary conditions for separability. Finding an analogy might prove very useful for the analysis of many-body correlations. Another important object in the theory of entanglement is the set of LOCC operations (local operations and classical communication), i.e., the operations that cannot create entanglement. In the case of pairing, the analogous set would contain passive operations and discarding modes. Are there other physical transformations that cannot create pairing? Do paired states, then, possibly allow us to implement such transformations similar to entanglement enabling non-LOCC operations?

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## APPENDIX A: USEFUL PROPERTIES OF SEPARABLE STATES

We give two technical lemmas that involve useful properties of product states.

### 1. Bound of $a_i^\dagger a_j^\dagger a_k a_l$+H.c. on separable states

In this section, we prove a bound of a special two-body operator on product states:

*Lemma A.1.* Let $\rho \in S_{\text{sep}}$ be a separable state. Then

$$|\text{tr}[(a_i^\dagger a_j^\dagger a_k a_l + \text{H.c.})\rho_s]| \leqslant \tfrac{1}{2}. \tag{A1}$$

*Proof.* Let $\mathcal{H}_{ijkl}$ be the Hilbert space spanned by $a_i^\dagger$, $a_j^\dagger$, $a_k^\dagger$, $a_l^\dagger$ and define $A_{ijkl}=a_i^\dagger a_j^\dagger a_k a_l$+H.c. Then $\text{tr}[A_{ijkl}\rho]=\text{tr}[\rho^{(ijkl)}A_{ijkl}]$, where $\rho^{(ijkl)}=\Sigma_{n=0}^{4}\beta_{ijkl}^{(n)}|n\rangle\langle n|$ is a mixed separable state according to Lemma II.2, and $|n\rangle$ denotes the occupation number basis for the subspace $\mathcal{H}_{ijkl}$. It is easily checked that $A_{ijkl}$ can have nonvanishing expectation value only for the two-particle state $|2\rangle=(\Sigma_{r=i,j,k,l}\mu_r a_r^\dagger)(\Sigma_{s=i,j,k,l}\nu_s a_s^\dagger)|0\rangle$. Using $|2\,\text{Re}(ab)|\leqslant|a|^2+|b|^2$ for any complex numbers $a$, $b$ and the normalization conditions $\Sigma_r|\mu_r|^2=\Sigma_r|\nu_r|^2=1$, one arrives at

$$\begin{aligned}|\text{tr}[A_{ijkl}\rho]| &= 2|\text{Re}[(\mu_i\nu_j-\mu_j\nu_i)(\mu_k\nu_l-\mu_l\nu_k)^*]| \\ &= (|\mu_i|^2+|\mu_j|^2)(|\mu_k|^2+|\mu_l|^2) \\ &\quad + (|\nu_i|^2+|\nu_j|^2)(|\nu_k|^2+|\nu_l|^2) \\ &\leqslant 0.25+0.25=0.5.\end{aligned}$$

■

### 2. Expectation values of one- and two-body operators for separable states

In this section, we will prove that the one- and two-body operators for separable states can be expressed in terms of matrix elements of projectors.

*Lemma A.2.* Let $\rho \in \mathcal{S}_{\text{sep}}^{(N)}$ be a pure separable state. Then

$$\langle n_i\rangle = P_{ii}, \tag{A2}$$

$$\langle a_i^\dagger a_j^\dagger a_k a_l\rangle_\rho = (P\otimes P)_{(ij)(lk)} - (P\otimes P)_{(ij)(kl)}, \tag{A3}$$

where $P=P^2=P^\dagger$ is a projector of rank $N$.

*Proof*. Consider $M$ modes. We go into the basis where the pure separable state is of the form $|\Phi\rangle=\Pi_{i=1}^N a_{\alpha_i}^\dagger|0\rangle$. In this basis $\langle a_{\alpha_i}^\dagger a_{\alpha_j}^\dagger a_{\alpha_k} a_{\alpha_l}\rangle_{|\Phi\rangle}=\delta_{il}\delta_{jk}-\delta_{ik}\delta_{jl}$, i.e., Eq. (A3) for $P=\mathrm{Id}_N$, where $\mathrm{Id}_N=\mathbb{1}_N\oplus 0_{M-N}\in\mathbb{C}^{M\times M}$. Now let $a_i^\dagger=\Sigma_k U_{ik}a_{\alpha_k}^\dagger$. Then

$$\begin{aligned}\langle a_i^\dagger a_j^\dagger a_k a_l\rangle_{\rho_s^{(N)}} &= (U\mathrm{Id}_N U^\dagger)\otimes(U\mathrm{Id}_N U^\dagger)_{(ij)(lk)} - (U\mathrm{Id}_N U^\dagger)\\ &\quad\otimes(U\mathrm{Id}_N U^\dagger)_{(ij)(kl)}\\ &= (P\otimes P)_{(ij)(lk)} - (P\otimes P)_{(ij)(kl)},\end{aligned}$$

and $P$ is a projector of rank $N$.

For the one-particle operators, we obtain $\langle n_i\rangle=P_{ii}$ as

$$\begin{aligned}(N-1)\langle n_i\rangle &= \Sigma_{j\neq i}\langle n_i n_j\rangle\\ &= \Sigma_{j\neq i}P_{ii}P_{jj} - |P_{ij}|^2\\ &= \Sigma_j P_{ii}P_{jj} - P_{ij}P_{ji}\\ &= \mathrm{tr}[P]P_{ii} - (P^2)_{ii}\\ &= (N-1)P_{ii}.\end{aligned}$$

■

## APPENDIX B: PROOF OF LEMMAS V.1 AND V.2

### 1. Proof of Lemma V.2

*Proof.* As $H_{1\pm}^{(p)}$, $H_{2\pm}^{(p)}$, $H_{3\pm}^{(p)}$ are built up of operators that are the product of at most two creation and annihilation operators, we can prove the lemma for separable states. In the first step, we will show that the three operators are positive on all separable states. Then we will show that all states within the set bounded by $H_{1\pm}^{(p)}$, $H_{2\pm}^{(p)}$, $H_{3\pm}^{(p)}$ correspond to a separable state. Finally we will show there exist states that are detected as paired by $H_{1\pm}^{(p)}$ and $H_{3\pm}^{(p)}$. Positivity of $H_{2\pm}^{(p)}$ on all number-conserving states will be shown in the proof of Lemma V.1 following below.

To show positivity of $H_{1\pm}^{(p)}$, $H_{2\pm}^{(p)}$, $H_{3\pm}^{(p)}$, it is sufficient to show the positivity for pure separable states, as the result for mixed states follows from convexity. From now on, let $\rho\in\mathcal{S}_{\mathrm{sep}}^{(N)}$.

#### *a.* $\mathrm{tr}[H_{1\pm}^{(p)}\rho]\geq 0$

In Lemma A.2 (see Appendix A), we have shown that the expectation values of number-conserving one- and two-body operators can be expressed in terms of matrix elements of projectors. Let $P$ be the rank $N$ projector such that $\langle a_i^\dagger a_j^\dagger a_k a_l\rangle_\rho=(P\otimes P)_{(ij)(lk)}-(P\otimes P)_{(ij)(kl)}$, $\langle n_i\rangle=P_{ii}$, and let $\tilde{P}=P|_{k-k,l,-l}$ the $4\times4$ principal submatrix of $P$ where the indices run over $k$, $-k$, $l$, $-l$. Then we have the following inequalities:

$$\langle n_k n_{-k}\rangle = P_{kk}P_{-k-k} - |P_{k-k}|^2 \leq \frac{1}{2}(|P_{kk}|^2+|P_{-k-k}|^2) - |P_{k-k}|^2, \tag{B1}$$

$$\begin{aligned}|\langle a_k^\dagger a_{-k}^\dagger a_{-l}a_l + \mathrm{H.c.}\rangle| &= 2|\mathrm{Re}(P_{kl}P_{-k-l} - P_{k-l}P_{-kl})| \qquad\text{(B2)}\\ &\leq 2(|P_{kl}||P_{-k-l}| + |P_{k-l}||P_{-kl}|)\\ &\leq (|P_{kl}|^2+|P_{-k-l}|^2+|P_{k-l}|^2+|P_{-kl}|^2).\end{aligned} \tag{B3}$$

These results imply

$$\mathrm{tr}[\rho H_{1\pm}^{(p)}] \geq \frac{1}{2}\mathrm{tr}[\tilde{P}-\tilde{P}^2] + |P_{k-k}|^2 + |P_{l-l}|^2. \tag{B4}$$

We use the inclusion principle [46], stating that the eigenvalues of an $r\times r$ principal submatrix $M_r$ of an $n\times n$ Hermitian matrix $M$ fulfill $\lambda_k(M)\leq\lambda_k(M_r)\leq\lambda_{k+n-r}(M)$, where the eigenvalues are arranged in increasing order. As $P$ is a projector, we have $0\leq\lambda_k(P)\leq\lambda_k(\tilde{P})\leq\lambda_{k+M-r}(P)\leq 1$. Hence,

$$\mathrm{tr}[H_{1\pm}^{(p)}\rho] \geq \frac{1}{2}\mathrm{tr}[\tilde{P}-\tilde{P}^2] \geq \frac{1}{2}\sum_k \lambda_k(\tilde{P})[1-\lambda_k(\tilde{P})] \geq 0. \tag{B5}$$

#### *b.* $\mathrm{tr}[H_{2\pm}^{(p)}\rho]\geq 0$

Define $O_1=n_k n_{-k}+n_l n_{-l}\geq 0$, $O_2^{\pm}=1\pm a_k^\dagger a_{-k}^\dagger a_{-l}a_l+\mathrm{H.c.}\geq 0$. Then $H_{2\pm}^{(p)}=O_1O_2^{\pm}$, and as $[O_1,O_2^{\pm}]=0$ we conclude that $H_{2\pm}^{(p)}=O_1O_2^{\pm}\geq 0$.

#### *c.* $\mathrm{tr}[H_{3\pm}^{(p)}\rho]\geq 0$

We will need the Lemma II.2: $\mathrm{tr}[H_{3\pm}^{(p)}\rho]=\mathrm{tr}[H_{3\pm}^{(p)}\rho_{kl}]$, where $\rho_{kl}=\Sigma_{n=0}^4\beta_n|n\rangle\langle n|$, $\beta_n\geq 0$, $\Sigma_{n=0}^4\beta_n=1$, and $|n\rangle$, $n=0,\ldots,4$ are separable $n$-particle states. Let $\langle H_{3\pm}^{(p)}\rangle_n=\langle n|H_{3\pm}^{(p)}|n\rangle$. Then a straightforward calculation leads to $\langle H_{3\pm}^{(p)}\rangle_0=1$, $\langle H_{3\pm}^{(p)}\rangle_1=\frac{1}{2}$, $\langle H_{3\pm}^{(p)}\rangle_2=\frac{1}{2}$, $\langle H_{3\pm}^{(p)}\rangle_3=0$, and $\langle H_{3\pm}^{(p)}\rangle_4=0$. Linearity of the trace implies $\mathrm{tr}[H_{3\pm}^{(p)}\rho]\geq 0$. Hence, all separable states lie within the set bounded by the planes defined by the witness operators $H_{1\pm}^{(p)}$, $H_{2\pm}^{(p)}$, $H_{3\pm}^{(p)}$.

Next, we show that each point within the polytope $C^{\mathrm{unpaired}}$ corresponds to a separable state. As $S_{\mathrm{sep}}$ is convex, it is sufficient to check that for every extreme point of $C^{\mathrm{unpaired}}$ there exists a separable state. This is indeed the case: The extreme points of $C^{\mathrm{unpaired}}$ are (0, 0, 0), (2, 0, 0), (4, 2, 0), $(2,1/2,\pm1/2)$, which correspond, for example, to the separable states $|0\rangle$, $a_k^\dagger a_l^\dagger|0\rangle$, $a_k^\dagger a_{-k}^\dagger a_l^\dagger a_{-l}^\dagger|0\rangle$, and $(a_k^\dagger+a_l^\dagger)(a_{-k}^\dagger\pm a_{-l}^\dagger)/2|0\rangle$, respectively.

It remains to show that $H_{1\pm}^{(p)}$ and $H_{3\pm}^{(p)}$ are pairing witnesses. Define $|\Psi\rangle=\frac{1}{\sqrt{2}}(a_k^\dagger a_{-k}^\dagger+a_l^\dagger a_{-l}^\dagger)|0\rangle$. Then $\mathrm{tr}[H_{1\pm}^{(p)}|\Psi\rangle\langle\Psi|]=\mathrm{tr}[H_{3\pm}^{(p)}|\Psi\rangle\langle\Psi|]=-1$. ■

### 2. Proof of Lemma V.2

*Proof.* It is sufficient to prove the lemma for $\rho\in\mathcal{S}(\mathcal{A}_N)$, as the result for a general number-conserving state follows from convexity.

#### *a.* $\mathrm{tr}[H_1\rho]\geq 0$

$H_1=\frac{1}{2}(n_k-n_{-k})^2+\frac{1}{2}(n_l-n_{-l})\geq 0.$

### *b.* $\mathrm{tr}[H_{2\pm}\rho]\geqslant 0$

Shown in the proof of Thm. V.2.

### *c.* $\mathrm{tr}[H_{3\pm}\rho]\geqslant 0$

Let $\rho_{kl}=\Sigma_{n=1}^{4}\beta_n|0\rangle\langle n|$ be the reduced density operator in the modes $\pm k$, $\pm l$. We can rewrite $H_{3\pm}$ in the form $H_3=2-\frac{1}{2}(n_k+n_{-k}+n_l+n_{-l})[1\mp(a_k^\dagger a_{-k}^\dagger a_{-l}a_l+\mathrm{H.c.})]$. Defining $O_{2\mp}=1\mp(a_k^\dagger a_{-k}^\dagger a_{-l}a_l+\mathrm{H.c.})$, we obtain $\langle O_{2\mp}\rangle_0=\langle O_{2\mp}\rangle_1=\langle O_{2\mp}\rangle_3=\langle O_{2\mp}\rangle_4=1$, $\langle O_{2\mp}\rangle_2\leqslant 2$. This implies $\mathrm{tr}[\rho H_{3\pm}]\geqslant 4-(\beta_1+2\beta_2+3\beta_3+4\beta_4)\geqslant 4-\Sigma_{n=0}^{4}n\beta_n=4-\mathrm{tr}[(n_k+n_{-k}+n_l+n_{-l})\rho_{kl}]\geqslant 0$

As in the proof of Lemma V.1, it remains to show that the extreme points of $C^{\mathrm{all}}$ correspond to some fermionic state. It has been shown in the proof of Lemma V.1 that (0, 0, 0), (2, 0, 0), and (4, 2, 0) can be reached by some separable state. The remaining two extreme points, $(2,1,\pm 1)$, correspond, for example, to the state $\frac{1}{\sqrt{2}}(a_k^\dagger a_{-k}^\dagger+a_l^\dagger a_{-l}^\dagger)|0\rangle$. ∎

## APPENDIX C: PROOF OF THM. V.4

In this section, we will provide all the details leading to Thm. v.4, starting with the bound on separable states:

*Lemma C.1*. Let $\rho\in S_{\mathrm{sep}}$ with $\mathrm{tr}[N_{\mathrm{op}}\rho]=N$ and let $H(\{v_k\})$ be as in Thm. V.4. Then $\mathrm{tr}[H(\{v_k\})\rho_s]\geqslant 0$.

*Proof*. The operator $H_k$ acts nontrivially only on the modes $a_k^\dagger$, $a_{-k}^\dagger$, $a_{k+M}^\dagger$, $a_{-(k+M)}^\dagger$. Denote by $\rho_k$ the reduced density operator obtained when tracing out all but these four modes. According to Lemma II.2, $\rho_k=\Sigma_{n=0}^{4}\beta_k^{(n)}|n\rangle\langle n|$ is a convex combination of separable $n$-particle states $|n\rangle\langle n|$. We proved in Lemma A.1 that $|\mathrm{tr}[(P_k^\dagger P_{k+M}+\mathrm{H.c.})\rho_s]|\leqslant 1/2$. Hence $\langle H(\{v_k\})\rangle\geqslant 2N(1-\epsilon)-2\Sigma_{k=1}^{M}(|v_k|^2\langle N_k\rangle+\beta_k^{(2)})$. Now $2\beta_k\leqslant\langle N_k\rangle\leqslant 4$ and $|v_k|^2\leqslant 1-\epsilon$ so that $|v_k|^2\ \langle N_k\rangle+\beta_k^{(2)})\leqslant 4$. Due to the particle number constraint $\Sigma_{k=1}^{M}\langle N_k\rangle=N$, this value can be taken for $k=1,\ldots,N/4$. Hence, $-2\Sigma_{k=1}^{M}(|v_k|^2\langle N_k\rangle+\beta_k^{(2)})\geqslant -2\times 4(1-\epsilon)N/4$ so that $\langle H(\{v_k\})\rangle\geqslant 0$. ∎

To show the witness character of $H(\{v_k\})$, we also have to prove that there exists a BCS state that is detected by the Hamiltonian. We will need the following theorem about the distribution described by the $|\lambda_N|^2$ in Eq. (16):

*Theorem C.2*. Let $|\Psi_{\mathrm{Gauss}}\rangle=\Sigma_{N=0}^{M}\lambda_N^{(M)}|\Psi_{\mathrm{BCS}}^{(N)}\rangle$ like in Eq. (15) and (17). If $\Sigma_{k=1}^{M}|u_k|^2|v_k|^2=O(N^\gamma)$ for some $\gamma>0$, then in the limit $N\to\infty$ the $|\lambda_N|^2$ converge to a normal distribution,

$$|\lambda_N|^2=\frac{1}{\sqrt{2\pi}\sigma_{\bar N}}\exp\left[-\frac{(N-\bar N)^2}{2\sigma_{\bar N}^2}\right], \tag{C1}$$

where $2\bar N=2\Sigma_{k=1}^{M}|v_k|^2$ is the mean particle number for the variational state, and the variance is given by $\sigma_{\bar N}^2=4\Sigma_{k=1}^{M}|v_k|^2|u_k|^2$.

*Proof*. For the proof we will need a theorem from probability theory known as Lyapunov's central limit theorem [63]:

*Theorem C.3*. (Lyapunov's central limit theorem). Let $X_1$, $X_2,\ldots$ be independent random variables with distribution functions $F_1$, $F_2,\ldots$, respectively, such that $EX_n=\mu_n$ and var $X_n=\sigma_n^2<\infty$, with at least one $\sigma_n>0$. Let $S_n=X_1+\ldots+X_n$ and $s_n=\sqrt{\mathrm{var}(S_n)}=\sqrt{\sigma_1^2+\ldots+\sigma_n^2}$. If the Lyapunov condition

$$\frac{1}{s_n^{2+\delta}}\sum_{k=1}^{n}E|X_k-\mu_k|^{2+\delta}\underset{n\to\infty}{\to}0$$

is satisfied for some $\delta>0$, then the normalized partial sums $\frac{S_n-ES_n}{s_n}$ converge in distribution to a random variable with normal distribution $N(0,1)$.

Consider the observables $X_k=n_k+n_{-k},k=1,\ldots,M$, where $n_{\pm k}=0,1$ is the number of particles with quantum numbers $\pm k$, respectively. The $X_k$ can be considered as classical random variables since they commute mutually. In the variational BCS state, the random variable $S_M=\Sigma_{k=1}^{M}X_k$ is distributed according to the probability distribution

$$P(S_M=2N)=\sum_{k_1<\cdots<k_M=1}^{M}|v_{k_1}|^2\cdots|v_{k_N}|^2|u_{k_{N+1}}|^2\cdots|u_{k_M}|^2$$
$$=\left(\prod_k|u_k|^2\right)\sum_{k_1<\cdots<k_M=1}^{M}\frac{|v_{k_1}|^2\cdots|v_{k_N}|^2}{|u_{k_1}|^2\cdots|u_{k_N}|^2} \tag{C2}$$

$$=\frac{|C|^2}{(N!)^2|C_N|^2}=|\lambda_N^{(M)}|^2. \tag{C3}$$

With the help of Thm. C.3 applied to the random variable $S_M$, we can now complete the proof of Thm. C.2, i.e., show that $\lambda_N^{(M)}$ converges to a normal distribution for large $M$. We start calculating the expectation value $\mu_k$ of $X_k$. For a BCS state, $X_k=0,2$, as particles with quantum numbers $\pm k$ always appear in pairs. As $P(X_k=0)=|u_k|^2$, $P(X_k=2)=|v_k|^2$, we get $\mu_k=2|v_k|^2$ and $E(S_M)=2\Sigma_k|v_k|^2\equiv 2\bar N$. For calculating the variance, note that $X_k^2=n_k^2+n_{-k}^2+2n_kn_{-k}=0,4$, and $P(X_k^2=0)=|u_k|^2$, $P(X_k^2=4)=|v_k|^2$. Hence

$$\mathrm{var}(X_k)=4|u_k|^2|v_k|^2,\quad s_M^2=4\sum_k|u_k|^2|v_k|^2. \tag{C4}$$

To apply the central limit theorem, we consider $E(|X_k-\mu_k|^4)$. Using $P(|X_k-\mu_k|^4=\mu_k^4)=|u_k|^2$, $P[|X_k-\mu_k|^4=(2-\mu_k)^4]=|v_k|^2$, and $\mu_k=2|v_k|^2$, we arrive at

$$E(|X_k-\mu_k|^4)=16|u_k|^2|v_k|^2(|u_k|^6+|v_k|^6)$$
$$\leqslant 16|u_k|^2|v_k|^2(|u_k|^2+|v_k|^2)$$
$$=16|u_k|^2|v_k|^2. \tag{C5}$$

Setting $\delta=2$ in the Lyapunov condition, we obtain

$$\frac{1}{s_M^4}\sum_{k=1}^{M}E(|X_k-\mu_k|^4)\leqslant\frac{4}{s_M^2}=O(N^{-\gamma})\to 0, \tag{C6}$$

where we have applied the assumption of the theorem $\Sigma_{k=1}^{M}|v_k|^2|u_k|^2=O(N^\gamma)$ in the last step. The central limit theorem implies that $S_M$ converges to a normal distribution with expectation values $2\bar N=2\Sigma_k|v_k|^2$ and variance $\sigma_{\bar N}^2=4\Sigma_k|v_k|^2|u_k|^2$. ∎

With this result at hand, we can prove the following:

*Lemma C.4*. Let $H(\{v_k\})$ and $|\Psi_{\mathrm{BCS}}^{(N)}\rangle$ be defined as in Thm. 5.4. If $\epsilon>18/\sqrt{\pi N}$, then

$$\langle\Psi_{\mathrm{BCS,sym}}^{(N)}|H(\{v_k\})|\Psi_{\mathrm{BCS,sym}}^{(N)}\rangle<0.$$

*Proof*. We will use the correspondence of variational and number-conserving BCS states, deriving first a bound for $|\langle H(\{v_k\})\rangle_{\rm var}-\langle H(\{v_k\})\rangle_N|$, where $|\Psi_{\rm Gauss}\rangle=\Sigma_{k=1}^{2M}\lambda_n|\Psi_{\rm BCS,sym}^{(n)}\rangle$ with $|\Psi_{\rm BCS,sym}^{(n)}\rangle$ like in Thm. 5.4. To do so, we will need that the $|\lambda_n|^2$ are normally distributed. From $|u_k|^2=1-|v_k|^2\geq\epsilon$, where $\epsilon>18/(\sqrt{2\pi\bar{N}})$ and $\Sigma_{k=1}^{2M}|v_k|^2=\bar{N}$, it follows that $\sigma_{\bar{N}}=\Sigma_{k=1}^{2M}|v_k|^2|u_k|^2\geq\epsilon\bar{N}=O(\sqrt{N})$. Hence, we know from Thm. C.2 that the $|\lambda_n|^2$ describe a normal distribution around $\bar{N}\approx N$ with standard deviation $\sigma_{\bar{N}}$.

Now, write $H(\{v_k\})=H_0-2W+2(1-\epsilon)\Sigma_{k=1}^{M}N_k$, where

$$H_0=-2\sum_{k=1}^{M}|v_k|^2N_k,$$

$$W=2\sum_k P_k^\dagger P_{k+M}+P_{k+M}^\dagger P_k.$$

We start with a bound for $|\langle H_0\rangle_{\rm var}-\langle H_0\rangle_N|\leq T_1+T_2$, where

$$T_1=\left|\sum_{\Delta\in[-\sigma_{\bar{N}}^2,\sigma_{\bar{N}}^2]}|\lambda_{N+\Delta}|^2(\langle H_0\rangle_{N+\Delta}-\langle H_0\rangle_N)\right|,$$

$$T_2=\left|\sum_{\Delta\notin[-\sigma_{\bar{N}}^2,\sigma_{\bar{N}}^2]}(|\lambda_{N+\Delta}|^2(\langle H_0\rangle_{N+\Delta}-\langle H_0\rangle_N)\right|. \quad \text{(C7)}$$

A bound for $T_2$ can be easily derived noting that

$$|\langle H_0\rangle_n-\langle H_0\rangle_{n'}|=8\left|\sum_k|v_k|^2(\langle n_k\rangle_n-\langle n_k\rangle_{n'})\right|, \quad \text{(C8)}$$

and for $n=N+\Delta>=N$ we have $\Sigma_k|v_k|^2(\langle n_k\rangle_n-\langle n_k\rangle_N)\leq\Sigma_k|v_k|^2\langle n_k\rangle_n\leq n$, as $|v_k|^2\leq 1$. Hence,

$$\begin{aligned}T_2&\leq 16\left|\sum_{\Delta\notin[0,\sigma_{\bar{N}}^2]}|\lambda_{N+\Delta}|^2|N+\Delta|\right|\\&\leq 8\frac{\sigma_{\bar{N}}}{\sqrt{2\pi}}e^{-\sigma_{\bar{N}}^2/2}+4N[1-\mathrm{erf}(\sigma_{\bar{N}}/\sqrt{2})]\\&\leq 8\frac{\sigma_{\bar{N}}}{\sqrt{2\pi}}+4N[1-\mathrm{erf}(\sigma_{\bar{N}}/\sqrt{2})], \quad \text{(C9)}\end{aligned}$$

where we have approximated the sum by an integral in the second step. For bounding $T_1$, we will show first that for $n=N+\Delta$, where $\Delta\in[-\sigma_{\bar{N}}^2,\sigma_{\bar{N}}^2]$, we have $\langle n_k\rangle_n-\langle n_k\rangle_{n-1}\geq 0$. Expanding the BCS wave function

$$|\Psi_{\rm BCS,sym}^{(n)}\rangle=C_n n!\sum_{j_1<\cdots<j_n=1}^{2M}\alpha_{j_1}\cdots\alpha_{j_n}P_{j_1}^\dagger\cdots P_{j_n}^\dagger|0\rangle, \quad \text{(C10)}$$

the expectation value of the number operator is easily calculated to be $\langle n_k\rangle_n=|C_n|^2(n!)^2|\alpha_k|^2S_k^{(n-1)}$, where

$$S_k^{(n)}=\sum_{\substack{j_1<\cdots<j_n=1\\ j_i\neq k}}^{2M}|\alpha_{j_1}|^2\cdots|\alpha_{j_n}|^2. \quad \text{(C11)}$$

If $0<|v_k|^2\leq 1-\epsilon$, there exists a lower bound on the coefficients $|\alpha_k|^2=|v_k|^2/\sqrt{1-|v_k|^2}\geq b\,\forall\,k$. Then $S_k^{(n-1)}$ and $S_k^{(n-2)}$ are related via

$$S_k^{(n-1)}\geq b\frac{2M-(n-1)}{n-1}S_k^{(n-2)}.$$

In the proof of Thm. C.2, we show that

$$\frac{|\lambda_n|^2}{|\lambda_{n-1}|^2}=\frac{|C_{n-1}|^2[(n-1)!]^2}{|C_n|^2(n!)^2}, \quad \text{(C12)}$$

resulting in

$$\langle n_k\rangle_n-\langle n_k\rangle_{n-1}\geq\left(b\frac{2M-(n-1)}{n-1}-\frac{|\lambda_n|^2}{|\lambda_{n-1}|^2}\right)\times|C_n|^2(n!)^2|\alpha_k|^2S_k^{(n-2)}. \quad \text{(C13)}$$

For $n=N+\Delta$ and $\Delta\in[-\sigma_N^2,\sigma_N^2]$, the normal distribution of the $|\lambda_n|^2$ implies $|\lambda_n|^2/|\lambda_{n-1}|^2=\exp[(2\Delta-1)/(2\sigma_{\bar{N}}^2)]\leq e$. Hence, $b\frac{2M-(n-1)}{n-1}-\frac{|\lambda_n|^2}{|\lambda_{n-1}|^2}\geq 0\Leftrightarrow b\geq e\frac{n}{2M-(n-1)}>3\frac{n-1}{2M-(n-1)}$. For $M=q(n-1)$, this is equivalent to $|\alpha_k|^2\geq 3/(2q-1)$, which can be achieved for $q\gg 1$. The last condition is satisfied, as we are considering dilute systems, where $M\gg\bar{N}$. Thus, $\langle n_k\rangle_n-\langle n_k\rangle_{n-1}\geq 0$, implying $\Sigma_k|v_k|^2(\langle n_k\rangle_n-\langle n_k\rangle_{n-1})\leq 1$, as $|v_k|^2\leq 1$. Using Eq. (C8) and a telescope sum, we conclude that

$$\begin{aligned}T_1&\leq 8\left|\sum_{\Delta\in[-\sigma_{\bar{N}},\sigma_{\bar{N}}]}|\lambda_{N+\Delta}|^2|\Delta|\right|\\&\leq 8\left|\sum_\Delta|\lambda_{N+\Delta}|^2|\Delta|\right|\\&=16\frac{\sigma_{\bar{N}}}{\sqrt{2\pi}}. \quad \text{(C14)}\end{aligned}$$

Next, we derive the bound for the operator $W$. Its expectation value is given by

$$\langle W\rangle_n=|C_n|^2(n!)^22\sum_k|\alpha_k|^2\sum_{\substack{j_1<\cdots<j_{n-1}\\ j_i\neq k,k+M}}^{2M}|\alpha_{j_1}|^2\cdots|\alpha_{j_{n-1}}|^2. \quad \text{(C15)}$$

For $n\in[N-\Delta,N+\Delta]$, we use the same argumentation we have used for bounding $\langle n_k\rangle_n-\langle n_k\rangle_{n-1}$, to obtain

$$\langle W\rangle_n-\langle W\rangle_{n-1}\leq 2. \quad \text{(C16)}$$

Further, $\langle n_k\rangle_n=\langle P_k^\dagger P_{k-M}^\dagger+\text{H.c.}\rangle_n/2+\langle n_kn_{k+M}\rangle_n$ due to the symmetry $\alpha_k=\alpha_{k+M}$. Hence, $\langle W\rangle_n\leq 2n$. Thus, up to a factor of 2 we obtain the same bound as for $H_0$. Putting all the pieces together, we find that

$$|\langle H(\{v_k\})\rangle_{\mathrm{var}} - \langle H(\{v_k\})\rangle_N| \leq 2(1-\epsilon) + \frac{72}{\sqrt{2\pi}}\sigma_N + 12N[1-\mathrm{erf}(\sigma_N/\sqrt{2})]. \tag{C17}$$

In the limit of large $x$, the error function $\mathrm{erf}(x/\sqrt{2\pi})$ can be approximated by the following formula:

$$1-\mathrm{erf}(x/\sqrt{2}) = 2\frac{\exp[-x^2/2]}{\sqrt{2\pi}}(x^{-1}-x^{-3}+\cdots). \tag{C18}$$

As $\sigma_N = O(\sqrt{N})$, we conclude

$$12N[1-\mathrm{erf}(\sigma_N^-/\sqrt{2})] \leq 24\sigma_N^- \exp[-\sigma_N^{2}/2]/(\epsilon\sqrt{2\pi}) \rightarrow 0$$

for $N \gg 1$. A straightforward calculation results in $\langle H(\{v_k\})\rangle_{\mathrm{var}} = -4N\epsilon$, leading immediately to the statement of the theorem. ■

## APPENDIX D: LEMMA FOR THE PROOF OF THM. 5.6

*Lemma D.1*. Every pure separable state $\rho \in \mathcal{S}(\mathcal{A}_N)$ fulfills $\sum_{kl=1}^{M} |\langle P_k^\dagger P_l\rangle_\rho| \leq N/2$, and this bound is tight.

*Proof*. Using Lemma A.2, we obtain

$$\sum_{k,l=1}^{M} |\langle P_k^\dagger P_l\rangle| = \sum_{k,l=1}^{M} |P_{kl}P_{-k-l} - P_{k-l}P_{-kl}|, \tag{D1}$$

where $P = P^2 = P^\dagger$ and $\mathrm{tr}[P] = N$. Using the triangle inequality, we get

$$\sum_{k,l=1}^{M} |\langle P_k^\dagger P_l\rangle| \leq \frac{1}{2}\sum_{k,l} (|P_{kl}|^2 + |P_{-k-l}|^2 + |P_{k-l}|^2 + |P_{-kl}|^2) = \frac{1}{2}\mathrm{tr}[P^2] = N/2.$$

In the last step, we have used the property that the sum of the squares of a normal matrix is equal to the sum of squares of its eigenvalues. Taking the square root, we obtain the bound of our claim.

The bound is tight, as $P = \mathbb{1}_{2_N}$ implies $\sum_{kl} |\langle P_k^\dagger P_l\rangle| = N/2$, which is obtained for $|\Phi\rangle = \Pi_{i=1}^{N} a_i^\dagger |0\rangle$. ■

## APPENDIX E: PROOF OF LEMMA 3.5

*Proof*. Let $|i,j\rangle = a_i^\dagger a_j^\dagger |0\rangle$ and consider the subspace spanned by the states $\{|k,-k\rangle, |l,-l\rangle, |k,l\rangle, |k,-l\rangle, |-k,l\rangle, |-k,-l\rangle\}$. In this basis, the two-particle RDO $\rho_2^{(N)}$ of $|\Psi_{\mathrm{BCS}}^{(N)}\rangle$ is of the form

$$\rho_2^{(N)} = \frac{1}{4+2a_1}\begin{pmatrix} a_1 & a_2 & 0 \\ a_2 & a_1 & 0 \\ 0 & 0 & \mathbb{1}_4 \end{pmatrix}, \tag{E1}$$

where $a_1 = (M-1)/(N-1)$, $a_2 = (M-N)/(N-1)$. The witness operator $H_1^{(p)}$ of Thm. 5.1 has a negative expectation value on $\rho_2^{(N)}$, hence the state is paired in these modes.

For solving the entanglement question, we will use the following theorem [25] applicable to mixed fermionic states of two particles each living on a single-particle Hilbert space of dimension 4:

*Theorem E.1*. Let the mixed state acting on $\mathcal{A}_4$ have a spectral decomposition $\rho = \sum_{i=1}^{r} |\Psi_i\rangle\langle\Psi_i|$, where $r$ is the rank of $\rho$, and the eigenvectors $|\Psi_i\rangle$ belonging to nonzero eigenvalues $\lambda_i$ are normalized as $\langle\Psi_i|\Psi_j\rangle = \lambda_i\delta_{ij}$. Let $|\Psi_i\rangle = \sum_{a,b} w_{ab} a_a^\dagger a_b^\dagger |0\rangle$ in some basis, and define the complex symmetric $r\times r$ matrix $C$ by

$$C_{ij} = \sum_{abcd} \epsilon^{abcd} w_{ab}^i w_{cd}^j, \tag{E2}$$

which can be represented using a unitary matrix as $C = UC_dU^T$, with $C_d = \mathrm{diag}[c_1, \ldots, c_r]$ diagonal and $|c_1| \geq |c_2| \geq \cdots \geq |c_r|$. The state has Slater number 1 if and only if

$$|c_1| \leq \sum_{i=2}^{r} |c_i|. \tag{E3}$$

The spectral decomposition of $\rho_2^{(N)}$ is given by

$$\rho_2^{(N)} = |\Psi_+\rangle\langle\Psi_+| + |\Psi_-\rangle\langle\Psi_-| + |\Psi_{kl}\rangle\langle\Psi_{kl}| + |\Psi_{k-l}\rangle\langle\Psi_{k-l}| + |\Psi_{-kl}\rangle\langle\Psi_{-kl}| + |\Psi_{-k-l}\rangle\langle\Psi_{-k-l}|,$$

where $|\Psi_+\rangle = \sqrt{\frac{a_+}{5+a_+}}|\psi_+\rangle$, $|\Psi_-\rangle = \sqrt{\frac{1}{5+a_+}}|\psi_-\rangle$, and $|\Psi_{\pm k,\pm l}\rangle = \sqrt{\frac{1}{5+a_+}}|\pm k, \pm l\rangle$. Here $|\psi_\pm\rangle = \frac{1}{\sqrt{2}}(|k,-k\rangle \pm |l,-l\rangle)$ and $a_+ = (2M-N-1)/(N-1)$. Defining $\gamma^2 = 1/(5+a_+)$, one obtains

$$C = \gamma^2 \begin{pmatrix} a_+ & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \tag{E4}$$

with spectrum $\mathrm{spec}(C) = \gamma^2\{a_+, 1, 1, -1, -1, -1\}$. For $M \leq N$, the state $|\Psi_{\mathrm{BCS}}^{(N)}\rangle$ is separable, so we can take $M > N$. Hence, $a_+\gamma^2$ is the eigenvalue with the biggest absolute value. According to Thm. E.1, the reduced state in the subspace of the four modes is entangled iff $|c_1| \leq \sum_{i=2}^{r} |c_i|$. For our example, this holds iff $M > 3N-2$. ■

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