

# Displaced Fermionic Gaussian States and their Classical Simulation

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Fermionic Gaussian operators have predominantly been explored within the confines of even Gaussian operators with zero mean. This work considers displaced Gaussian operators with nontrivial linear terms, leading to a broader applicability of fermionic Gaussian theory. We provide an efficient classical simulation protocol for displaced Gaussian circuits and demonstrate their computational equivalence to circuits composed of nearest-neighbor matchgates augmented by single-qubit gates on an initial line. Additionally, we construct a novel unitary embedding that maps  $n$ -qubit displaced Gaussian states into  $(n + 1)$ -qubit even Gaussian states. This embedding facilitates the extension of existing Gaussian testing protocols to displaced Gaussian states and unitaries. Our results provide new tools for analyzing fermionic systems beyond the constraints of parity super-selection, enhancing both the theoretical understanding and practical simulation of fermionic computation.

## I. INTRODUCTION

Fermionic Gaussian operators form a crucial interface between physics, computation, and mathematics. In physics, fermionic Gaussian states correspond to free fermions, which arise in a variety of systems, such as the 1-dimensional Ising model and fermionic linear optics, where beam splitters and phase shifters act on non-interacting electrons [1]. These states are also foundational in computational chemistry, notably within the Hartree-Fock method for modeling molecular orbitals [2]. From a computational standpoint, fermionic Gaussian states underpin the framework of matchgate computation, one of the few known models enabling efficient classical simulation of quantum computations [3]. Mathematically, the Gaussian character of these operators connects to the tractability of Gaussian integrals over Grassmann variables [4–6]. Similar Gaussian structures also support classical simulation in bosonic systems, notably stabilizer states and Clifford unitaries [7–9].

In fermionic systems, Gaussian unitaries are generated by quadratic Hamiltonians without linear terms, reflecting the dynamics of non-interacting fermions. A parity super-selection rule in physical fermionic systems constrains states to definite parity and excludes Hamiltonians with odd terms [10, 11]; this constraint is also linked to the symmetry of fermion number conservation, whose observable manifests as the parity operator. Consequently, the study of fermionic Gaussian computation has predominantly focused on even Gaussian operators, which also conveniently exhibit a more manageable mathematical structure due to commutativity properties. However, in representations of fermionic algebra on non-fermionic platforms, such as 1-dimensional spin chains or qubit systems via the Jordan-Wigner transformation, the parity super-selection rule is more a mathematical convenience than physical necessity. It limits the scope

of Gaussian analysis by excluding certain operators and states; this impacts applications like fermionic convolution and variational characterizations Gaussianity [12].

This work addresses the limitations of conventional fermionic Gaussian theory imposed by the parity super-selection rule. To broaden the applicability of Gaussian theory in fermionic systems, we focus on displaced Gaussian states and unitaries—those with nontrivial linear terms in addition to quadratic ones. A high-level mathematical reduction, connecting the Lie algebras of displaced and even Gaussian operators, was proposed in [13], and displaced Gaussian operators have explored in terms of their channel capacities [14]. However, a framework linking displaced Gaussian computation with the more extensively studied even Gaussian (or matchgate) computation remains undeveloped. This gap is significant given that even Gaussian computation has been deeply investigated in areas such as magic states, simulability, and resource theory [15–19]. Throughout this work, we use “Gaussian” to refer specifically to zero-mean cases, reserving “displaced Gaussian” for the general non-zero mean scenarios.

This work extends the scope of fermionic Gaussian theory by examining displaced Gaussian operators and situating them within the broader landscape of even Gaussian operators. A central challenge motivating this study is the ambiguity in defining displaced Gaussian states across differing interpretations of Gaussianity. Definitions of even Gaussian states vary by context: some computational works define them as the orbit of computational basis states under Gaussian unitaries [18, 20], while other physics-motivated works identify them as the thermal states of quadratic Hamiltonians [2, 21]. An alternative approach rooted in phase-space analysis characterizes Gaussian states by the quadratic form of their Grassmann representations [4, 14]. Extending these definitions to displaced Gaussian states raises consistency challenges. Though prior work on the Lie algebra embeddings of displaced Gaussian computation has suggested the classical simulability of such operators by generating a subalgebra of polynomial dimension [13], an explicit reduction from displaced to even Gaussian computation

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has yet to be fully articulated.

The main deliverables of this work are as follows: first, we unify the displaced extensions of the aforementioned definitions of even Gaussian states. Second, we introduce an efficient classical simulation algorithm for displaced Gaussian circuits and demonstrate that displaced Gaussian computation is generated by nearest-neighbor matchgates augmented with single-qubit gates on the initial line. Finally, we construct a novel unitary embedding that maps displaced Gaussian states into even Gaussian states, providing a bridge between the study of even and displaced fermionic Gaussian operators. Leveraging this embedding, we extend recent findings [12] to develop operational tests for identifying classically simulable displaced Gaussian states and unitaries.

Section II introduces displaced Gaussian operators and provides a review of the Jordan-Wigner transformation, matchgates, and existing results for even fermionic Gaussian operators. Section III examines the main properties of displaced Gaussian unitaries and states. Section IV presents a simulation protocol for displaced Gaussian circuits, highlighting the practical implications of our findings. Finally, Section V details the construction of the even Gaussian embedding and illustrates its application in constructing tests for displaced Gaussian components.

## II. PRELIMINARIES

A system of  $n$  fermionic modes is associated with  $2n$  Hermitian, traceless and Majorana operators  $\{\gamma_j\}_{j=1}^{2n}$  which generate a Clifford algebra  $\mathcal{C}_{2n}$  according to the anticommutation relations

$$\{\gamma_j, \gamma_k\} = 2\delta_{jk}I. \quad (\text{II.1})$$

They are related to the real and imaginary parts of the creation and annihilation operators by

$$\gamma_{2j-1} = a_j + a_j^\dagger, \quad \gamma_{2j} = i(a_j - a_j^\dagger). \quad (\text{II.2})$$

Using the Jordan-Wigner transform [22], the Majorana operators can also be identified with products of Pauli operators on the operator space  $\mathcal{H}_n$  of  $n$  qubits:

$$\begin{aligned} \gamma_{2j-1} &= Z^{\otimes(j-1)} \otimes X \otimes I^{\otimes(n-j)}, \\ \gamma_{2j} &= Z^{\otimes(j-1)} \otimes Y \otimes I^{\otimes(n-j)}. \end{aligned} \quad (\text{II.3})$$

Since permuting the tensor products does not change the anticommutation relations, the representation remains valid if we permute the qubits  $1, \dots, n$ . We identify the *initial line* of the circuit with the first subspace in equation II.3, and two qubits are *nearest neighbors* if they are adjacent in the tensor product.

Given an ordered subset (multi-index)  $J \subset [2n]$ , we denote the size of the subset  $J$  by  $|J|$  and define  $\gamma_J$  to be the ordered product  $\gamma_J = \prod_{j \in J} \gamma_j$  indexed by  $J$ . The products  $\{\gamma_J\}_{J \subset [2n]}$  form an orthonormal basis, so every

operator  $A \in \mathcal{C}_{2n} \cong \mathcal{H}_n$  has a Majorana expansion

$$A = \frac{1}{2^n} \sum_{J \subset [2n]} A_J \gamma_J, \quad A_J = \text{Tr}(\gamma_J^\dagger A) \in \mathbb{C}. \quad (\text{II.4})$$

The coefficients  $\{A_J\}$  are also called the “moments” of  $A$ . It is also useful to introduce  $2n$  self-adjoint Grassmann generators  $\{\eta_j\}_{j=1}^{2n}$  which generate a Grassmann algebra by the anticommutation relation  $\{\eta_j, \eta_k\} = 0$ . The Fourier transform  $\Xi_A(\eta) \in \mathcal{G}_{2n}$  is computed by multiplying  $2^n$  and substituting the generators in equation II.4, with  $\eta_J$  defined analogously:

$$\Xi_A(\eta) = \sum_{J \subset [2n]} A_J \eta_J. \quad (\text{II.5})$$

We identify the mean and the covariance of an operator  $A \in \mathcal{C}_{2n}$  with the first and second-order moments  $\{A_J\}_{j=1}^{2n} = \{\mu(A)_j\}$ ,  $\{A_{jk}\}_{j,k=1}^{2n} = \{\Sigma(A)_{jk}\}$ . These define the antisymmetric *extended covariance matrix* of  $A$

$$\tilde{\Sigma}(A) = \begin{bmatrix} \Sigma(A) & i\mu(A) \\ -i\mu(A)^T & 0 \end{bmatrix} \in \mathfrak{so}(2n+1, \mathbb{C}). \quad (\text{II.6})$$

Note that  $\tilde{\Sigma}(\rho), \Sigma(\rho)$  are purely imaginary for a Hermitian state  $\rho$ . They are normalized so that  $\Sigma(\rho \otimes I) = \Sigma(\rho) \oplus 0_{2 \times 2}$ . It is also convenient to define the raw extended covariance matrix

$$\bar{\Sigma}(A) = \frac{1}{2^n} \tilde{\Sigma}(A). \quad (\text{II.7})$$

Given a multi-index  $J \subset [2n+1]$ , we denote the  $|J| \times |J|$  antisymmetric matrix restriction of  $\tilde{\Sigma}(J)$  onto the subspaces indexed by  $J$  according to

$$[\tilde{\Sigma}(\rho)_{|J}]_{ab} = \tilde{\Sigma}(\rho)_{J_a J_b}. \quad (\text{II.8})$$

**Definition II.1** (displaced Gaussian unitary).  $U \in \mathcal{C}_{2n}$  is a *displaced Gaussian unitary* if

$$U = \exp \left( \frac{1}{2} \gamma^T h \gamma + i d^T \gamma \right) \quad (\text{II.9})$$

where  $h = \Sigma(\log U) \in \mathfrak{so}(2n, \mathbb{R})$  is real, antisymmetric and  $d \in \mathbb{R}^{2n}$ . It is a (even) Gaussian unitary if  $d = 0$ .

We denote the group of even or displaced Gaussian unitaries on  $n$  qubits by  $G(n)$  or  $DG(n) \subset \mathcal{C}_{2n}$ , respectively. It is known that  $U \in G(n)$  conjugates the Majorana operators by a rotation [23, Theorem 3]:

$$U \gamma_j U^\dagger = \sum_{k=1}^{2n} R_{kj} \gamma_k, \quad R = \exp [2 \bar{\Sigma}(\log U)]. \quad (\text{II.10})$$

Here  $\log U = iH$  is understood to be quadratic in the Majorana operators. Among the Gaussian unitaries, a special subset which only act nontrivially on two nearest-neighbor lines are called *nearest-neighbor matchgates*, or n.n matchgates. Every Gaussian unitary on  $n$  lines has

a local circuit decomposition into  $O(n^3)$  n.n matchgates ([23], Theorem 5). In light of equation II.10, the n.n. matchgates effect rotations which act nontrivially on subspaces  $4m-3, \dots, 4m$  or  $4m-1, \dots, 4m+2$  for some  $m$ .

The following definition can be found in [14]. Observe that  $iM = \mu(\rho)$  and  $d = \mu(\rho)$ .

**Definition II.2** (displaced Gaussian state). *A  $n$ -qubit state  $\rho \in \mathcal{C}_{2n}$  is a displaced Gaussian state if its Fourier transform admits a Gaussian expression:*

$$\Xi_\rho(\eta) = \exp\left(\frac{i}{2}\eta^T M \eta + d^T \eta\right) \quad (\text{II.11})$$

where  $M \in \mathfrak{so}(2n, \mathbb{R})$  and  $d \in \mathbb{R}^{2n}$ . It is a (even) Gaussian state if its mean  $d = 0$ .

We denote the set of even and displaced Gaussian states by  $\mathbf{Gauss}(n)$  and  $\mathbf{DGauss}(n) \subset \mathcal{C}_{2n}$ , respectively. A displaced Gaussian state is completely characterized by its extended covariance matrix (equation II.6). A special class of *diagonalized Gaussian states* consists of separable products of computational basis states: for some set of  $\lambda_j \in [-1, 1]$ ,

$$\rho_D = \bigotimes_{j=1}^n \frac{1 + \lambda_j Z}{2}, \quad \Sigma(\rho_D) = \bigoplus_{j=1}^n \begin{pmatrix} 0 & \lambda_j \\ -\lambda_j & 0 \end{pmatrix}. \quad (\text{II.12})$$

Given  $A \in \mathfrak{so}(2n, \mathbb{C})$ , there exists  $\rho \in \mathbf{Gauss}(n)$  such that  $\Sigma(\rho) = A$  if and only if  $-A^T A \leq I$  [4].

### III. DISPLACED GAUSSIAN THEORY

In this part we describe the main results about displaced Gaussian states and unitaries which generalize the even Gaussian counterparts. In particular, we see that every  $\rho \in \mathbf{DGauss}(n)$  is identified with the antisymmetric extended covariance  $\tilde{\Sigma}$ , upon which  $U \in DG(n)$  conjugates by a rotation. These results rigorously substantiate the intuition that the nonzero mean of displaced Gaussian operators can be effectively treated as the covariance on one more mode.

One advantage of defining Gaussian states according to its Fourier property is that expanding the exponential in equation II.11 yields the following extended Wick's formula. Recall equation II.8 for the following result: given  $J \subset [2n]$ , let  $\bar{J} = J \cup \{2n+1\}$  if  $|J|$  is odd else  $J$ ; also define the scalar factor  $\alpha_{|J|} = (-i)^{|J| \bmod 2}$ .

**Proposition III.1.** *Every  $\rho \in \mathbf{DGauss}(n)$  satisfies*

$$\rho = \frac{1}{2^n} \sum_{J \subset [2n]} \alpha_{|J|} \text{Pf} \left[ \tilde{\Sigma}(\rho)_{|\bar{J}} \right] \gamma_J. \quad (\text{III.1})$$

A combinatorial proof is provided in Appendix B. Using the Lie algebra embedding identified by Knill [13], we derive the formula for  $U \gamma_J U^\dagger$  where  $U \in DG(n)$ .

In combination with Wick's formula, this yields the following displaced generalization of equation II.10. Here  $\log U = iH$  is proportional to the Hamiltonian quadratic in the Majorana operators, and  $\tilde{\Sigma}$  denotes the raw extended covariance matrix in equation II.7.

**Theorem III.2.** *Given  $U \in DG(n)$ ,  $\rho \in \mathbf{DGauss}(n)$  where  $H$  is quadratic in the Majorana operators, the extended covariance of  $U \rho U^\dagger \in \mathbf{DGauss}(n)$  is*

$$\tilde{\Sigma}(U \rho U^\dagger) = R \tilde{\Sigma}(\rho) R^T, \quad R = e^{2\tilde{\Sigma}(\log U)}. \quad (\text{III.2})$$

The detailed proof can be found in Appendix C. The main insight here is that under  $DG(n)$ , Majorana monomials of odd degree  $2m-1$  transform like an even monomial of degree  $2m$  on one more mode; in particular, the linear term  $\mu_j \gamma_j$  of a displaced Gaussian operator transforms as the covariance term  $i\mu_j \gamma_j \gamma_{2n+1}$ .

Even Gaussian states have been defined as those admitting a Gaussian Fourier expression [4, 14], the orbit of computational basis states under  $G(n)$  [18, 20], or thermal states of purely quadratic Hamiltonians [2, 21]. Our definition of  $\mathbf{DGauss}$  extends the first definition, yet it is equally plausible to adopt the displaced extensions of the circuit or thermal state definitions. Using theorem III.2, we show in Appendix D that all three definitions are in fact the same. This characterization bridges the physical, computational, and mathematical properties of displaced Gaussian states.

**Theorem III.3.**  *$\rho \in \mathcal{C}_{2n}$  is a displaced Gaussian state (equation II.11) iff it satisfies any of the following:*

1. **Thermal state:** *there exists a quadratic Hamiltonian  $H \in \mathcal{C}_{2n}$  such that  $\rho$  is its thermal state:*

$$\rho = \frac{e^{-H}}{\text{Tr}(e^{-H})}, \quad H = \frac{i}{2} \gamma^T h \gamma + d^T \gamma. \quad (\text{III.3})$$

Here  $h \in \mathfrak{so}(2n, \mathbb{R})$  is real antisymmetric and  $d \in \mathbb{R}^{2n}$ . A pure state  $\rho$  is a displaced Gaussian state iff it is the ground state of some  $H$  of the form above.

2. **Circuit output:**  *$\rho$  results from applying a displaced Gaussian unitary  $U_G \in DG(n)$  to a diagonalized Gaussian state  $\rho_D$ , i.e.  $\rho = U_G \rho_D U_G^\dagger$ .*

The proof proceeds by first establishing the desired equivalence for diagonalized Gaussian states (equation II.12), then extending to  $\mathbf{DGauss}(n)$  by showing that every such state can be diagonalized by an element of  $DG(n)$  using theorem III.2. One immediate corollary is the necessary and sufficient conditions for an antisymmetric matrix to be the extended covariance of some  $\rho \in \mathbf{DGauss}(n)$ . This extends the condition established for even Gaussian states in [4].

**Corollary III.1.**  *$A \in \mathfrak{so}(2n+1, \mathbb{C}) = \tilde{\Sigma}(\rho_G)$  for some  $\rho_G \in \mathbf{DGauss}(n)$  iff  $A$  has rank  $2n$  and there exists  $R \in SO(2n+1)$  such that  $RA^2 R^T \leq I_{2n+1}$ , the associated  $\rho_G$  is pure iff the nonzero eigenvalues of  $A^2$  are all 1.*

#### IV. CLASSICAL SIMULATION

One important reason to study displaced Gaussian unitaries is that they yield a larger class of efficiently classically simulable quantum circuits. The circuit characterization of  $\mathbf{DGauss}(n)$  in theorem III.3 also relates the study of displaced Gaussian unitaries to the study of displaced Gaussian states. In this section, we show that displaced Gaussian circuits are equivalent to n.n. matchgates augmented with single-qubit gates on the initial line. We also describe the efficient classical simulation of displaced Gaussian circuits. Detailed derivations can be found in Appendix E.

**Theorem IV.1.** *Every displaced Gaussian unitary  $U \in \mathbf{DG}(n)$  is the product of  $O(n^3)$  matchgates or single-qubit gates on the initial line of the circuit.*

Recall theorem III.2. A quadratic term  $\gamma_j \gamma_k$  for  $1 \leq j < k \leq 2n$  in the Hamiltonian generates rotation between the  $j$  and  $k$ -th subspaces of the extended covariance matrix. On the initial line of the Jordan-Wigner transform,  $R_X(\theta)_1$  corresponds to  $\gamma_1 = X_1$  in the Hamiltonian, which generates rotation between the first and  $(2n+1)$ -th subspaces of the extended covariance matrix. Every rotation in  $\mathbb{R}^{2n+1}$  can be decomposed into  $O(n^3)$  rotations generated by n.n. matchgates or  $R_X(\theta)_1$ .

In light of the circuit characterization in theorem III.3, displaced Gaussian states can be understood as the orbit of separable computational basis mixtures under  $\mathbf{DG}(n)$ . By slightly adapting the technique from [24, Theorem 3], we obtain the following result:

**Proposition IV.2.** *Every  $n$ -qubit product state is a displaced Gaussian state.*

To complete efficient simulation, it remains to simulate measurements. This is facilitated by applying Grassmann integral techniques for Gaussian integrals, as developed in [4–6]. In particular, we can efficiently simulate computational basis measurements on any subset of qubit lines. Given a subset  $K \subset [n]$  of lines to measure, where  $|K| = k$ , and a bit string  $x \in 0, 1^k$ , the associated measurement operator is defined as follows:

$$O(K, x) = \frac{1}{2^k} \prod_{j=1}^k I + (-1)^{x_j} Z_{K_j}. \quad (\text{IV.1})$$

This operator acts as  $|x\rangle\langle x|$  on the qubit lines indexed by  $K$ , while it applies the identity  $I$  on all other lines.

**Lemma IV.3.** *Given  $\rho \in \mathbf{DGauss}(n)$ , the expectation value of measuring  $O(K, x)$  is*

$$\text{Tr}[O(K, x)\rho] = \frac{1}{2^k} \sqrt{\det[1 + \Sigma(\rho)M]} \quad (\text{IV.2})$$

where  $M = \Sigma[2^{n-k}O(K, x)]$  is the covariance matrix of the even Gaussian state proportional to  $O$ .

Given a displaced Gaussian state as input, the effect of displaced Gaussian unitaries can be determined via theorem III.2, and the measurement outcomes in the computational basis can be computed using lemma IV.3.

**Theorem IV.4.** *A circuit consisting of displaced Gaussian unitaries, a displaced Gaussian state input, and computational basis measurements on any subset of qubit lines is efficiently classically simulable.*

Since both n.n. matchgates and single-qubit gates acting on the first line are displaced Gaussian unitaries, and product states qualify as displaced Gaussian states, we can conclude the following:

**Corollary IV.1.** *A circuit comprising n.n. matchgates and single-qubit gates on the first line, with a product state input and computational basis measurements on any subset of qubit lines, is efficiently classically simulable.*

As discussed in [16, 24], there exists several different classical simulation protocols for matchgate computation with different configurations. For instance, Jozsa and Miyake’s approach [23] exploits the degree-preserving property of Gaussian rotations in equation II.10 simulate product state inputs and measurements on a constant number of qubits. Alternatively, the method introduced by Valiant [3], later extended by Terhal and DiVincenzo [25], leverages the algebraic properties of fermionic operators to express state-measurement overlaps as the Pfaffians of cleverly constructed matrices, simulating an arbitrary number of measurement with computational basis state inputs, later generalized to product-state inputs by Brod [24]. Bravyi’s works provide another perspective by expressing overlaps as tractable, well-studied Gaussian Grassmann integrals [4, 5]. Extending this framework to displaced Gaussian operators offers a cohesive perspective that both lifts the parity super-selection constraint and implies the previous simulation protocols.

#### V. DISPLACED GAUSSIAN TESTING

Previous works have examined a channel embedding that maps  $\rho \in \mathbf{DGauss}(n)$  to  $\rho' \in \mathbf{Gauss}(n+1)$  [13, 14]. Such embeddings are fundamental to extending even Gaussian properties to displaced Gaussian states. However, this channel is not purity-preserving, as  $S(\rho') = S(\rho) + 1$ , where  $S(\rho)$  denotes the von Neumann entropy in bits. This lack of purity invariance poses challenges for extending computational protocols that rely on purity, such as the fermionic Gaussian test in [12].

In this section, we introduce the first construction of a unitary embedding,  $\mathcal{E} : \mathbf{DGauss}(n) \rightarrow \mathbf{Gauss}(n+1)$ . Leveraging this embedding, we develop operational protocols for testing displaced Gaussian states and unitaries.

**Definition V.1** (even embedding channel). *We define the even embedding channel  $\mathcal{E} : \mathcal{C}_{2n} \rightarrow \mathcal{C}_{2n+2}$  by*

$$\mathcal{E}(\rho) = V(\rho \otimes |+\rangle\langle +|)V^\dagger. \quad (\text{V.1})$$



Here  $V \in DG(n+1)$  is the displaced Gaussian unitary on  $n+1$  lines

$$V = \exp\left(-i\frac{\pi}{4}\gamma_{2n+2}\right). \quad (\text{V.2})$$

In Appendix F, we derive the following results and show how  $V$  can be implemented by elementary gates. We show that  $\mathcal{E}$  preserves Gaussianity as well as purity. Given the  $(2n+1)$ -sized extended covariance matrix  $\tilde{\Sigma}(\rho)$  of an  $n$ -qubit state  $\rho$ , by a standard matrix theorem [26] there exists a rotation  $R$  such that for each  $\lambda_j \in [-1, 1]$ ,

$$R\tilde{\Sigma}(\rho)R^T = \left[ \bigoplus_{j=1}^n \begin{pmatrix} 0 & -i\lambda_j \\ i\lambda_j & 0 \end{pmatrix} \right] \oplus (0). \quad (\text{V.3})$$

Block-decompose  $R$  into  $R_0 \in \mathbb{R}^{2n \times 2n}$ ,  $c \in \mathbb{R}$ , and  $s, r \in \mathbb{R}^{2n}$  so that  $R = \begin{bmatrix} R_0 & s \\ r^T & c \end{bmatrix}$ . We obtain the following result:

**Theorem V.1.** *An  $n$ -qubit state  $\rho \in \mathbf{DGauss}(n)$  iff  $\mathcal{E}(\rho) \in \mathbf{Gauss}(n+1)$ . The embedded covariance is*

$$\Sigma[\mathcal{E}(\rho)] = \begin{bmatrix} \Sigma(\rho) & -ir & i\mu(\rho) \\ ir^T & 0 & ic \\ -i\mu(\rho)^T & -ic & 0 \end{bmatrix} \in \mathfrak{so}(2n+2, \mathbb{C}). \quad (\text{V.4})$$

The even embedding for states has a counterpart for unitaries: given an  $n$ -qubit unitary  $U \in \mathcal{C}_{2n}$ , define

$$\tilde{U} = V(U \otimes I)V^\dagger \in \mathcal{C}_{2n+2}. \quad (\text{V.5})$$

The two embeddings are compatible by the equation

$$\mathcal{E}(U\rho U^\dagger) = \tilde{U}\mathcal{E}(\rho)\tilde{U}^\dagger.$$

**Lemma V.2.** *For every  $n$ -qubit unitary  $U$ ,*

$$U \in DG(n) \iff \tilde{U} \in G(n+1). \quad (\text{V.6})$$

Given  $U$  as in equation II.9,  $\tilde{U}$  is given by

$$\tilde{U} = \exp\left(\frac{1}{2}\gamma^T \tilde{h} \gamma\right), \quad \tilde{h} = \begin{bmatrix} h & 0_{2n \times 1} & -d \\ 0_{1 \times 2n} & 0 & 0 \\ d^T & 0 & 0 \end{bmatrix}. \quad (\text{V.7})$$

We now proceed to displaced Gaussian testing. One important tool in the study of fermionic Gaussian states is fermionic convolution [12]. The  $n$ -qubit convolution unitary acting  $2n$  qubits is defined by

$$W = \exp\left(\frac{\pi}{4} \sum_{j=1}^{2n} \gamma_j \gamma_{2n+j}\right) \in \mathcal{C}_{4n}. \quad (\text{V.8})$$

The fermionic convolution of two *even* states  $\rho, \sigma$  is

$$\rho \boxtimes \sigma = \text{Tr}_2[W(\rho \otimes \sigma)W^\dagger]. \quad (\text{V.9})$$

Here  $\text{Tr}_2$  denotes partial trace over the registers of  $\sigma$ . Fermionic convolution provides valuable tests for Gaussian states and unitaries. We denote by  $\rho_{\mathcal{E}}$  the fermionic

maximally entangled state, as defined in [4, Definition 6]. Our focus is on cases where  $|\psi\rangle$  and  $U$  (with  $U \in \mathcal{C}_{2n}$ ) are both *even* operators, leading to the following results:

1. **Gaussian State Test:** A state  $|\psi\rangle$  is Gaussian iff the overlap  $\langle\psi|(|\psi\rangle \boxtimes |\psi\rangle) = 1$ . This overlap is experimentally accessible through the swap test.
2. **Gaussian Unitary Test:** A unitary  $U$  is Gaussian iff its Choi state  $(U \otimes I_n)\rho_{\mathcal{E}}(U^\dagger \otimes I_n) \in G(n)$ .

Using Gaussianity-preserving properties established in theorem V.1 and lemma V.2, we obtain tests for the classically simulable displaced Gaussian components.

**Theorem V.3.** *For any  $n$ -qubit  $\rho, U \in \mathcal{C}_{2n}$ :*

- $\rho \in \mathbf{DGauss}(n)$  iff  $\mathcal{E}(\rho)$  passes the test for even Gaussian states.
- $U \in DG(n)$  iff  $V(U \otimes I)V^\dagger$  passes the test for even Gaussian unitaries.

## VI. CONCLUSION AND DISCUSSION

In this work, we presented foundational tools and results on displaced Gaussian states and their computational significance, expanding the conventional scope of fermionic Gaussian computations by encompassing circuits not limited by the fermionic parity constraint. The significance of displaced Gaussian states in the matchgate framework is highlighted by their close relation to well-studied even Gaussian circuits.

We characterized displaced Gaussian circuits as nearest-neighbor matchgates augmented with single-qubit gates on the initial line, unified physically and computationally motivated characterizations of displaced Gaussian states, and provided an simulation protocol for displaced Gaussian circuits as well as a unitary embedding of displaced Gaussian states. These results solidify displaced Gaussian operators as a pivotal class within matchgate computations.

Future directions may involve extending classical simulability to more flexible circuit topologies, such as allowing single-line gates on non-initial lines. Additionally, the complexity of linking displaced and even fermionic Gaussian computation motivates further theoretical study of particle-number symmetry's role in classical simulation, with potential applications to simulation protocols inspired by other physical particle types.

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- [1] D. P. DiVincenzo and B. M. Terhal, Fermionic linear optics revisited, *Foundations of Physics* **35**, 1967 (2005).
  - [2] J. Surace and L. Tagliacozzo, Fermionic gaussian states: an introduction to numerical approaches, *SciPost Physics Lecture Notes*, 054 (2022).
  - [3] L. G. Valiant, Quantum computers that can be simulated classically in polynomial time, in *Proceedings of the thirty-third annual ACM symposium on Theory of computing* (2001) pp. 114–123.
  - [4] S. Bravyi, Lagrangian representation for fermionic linear optics, *Quantum Info. Comput.* **5**, 216–238 (2005).
  - [5] S. Bravyi, D. Browne, P. Calpin, E. Campbell, D. Gosset, and M. Howard, Simulation of quantum circuits by low-rank stabilizer decompositions, *Quantum* **3**, 181 (2019).
  - [6] D. E. Soper, Construction of the functional-integral representation for fermion green’s functions, *Physical Review D* **18**, 4590 (1978).
  - [7] C. Weedbrook, S. Pirandola, R. García-Patrón, N. J. Cerf, T. C. Ralph, J. H. Shapiro, and S. Lloyd, Gaussian quantum information, *Reviews of Modern Physics* **84**, 621 (2012).
  - [8] K. Bu, W. Gu, and A. Jaffe, Quantum entropy and central limit theorem, *Proceedings of the National Academy of Sciences* **120**, e2304589120 (2023).
  - [9] K. Bu, W. Gu, and A. Jaffe, Discrete quantum gaussians and central limit theorem, *arXiv:2302.08423* (2023).
  - [10] K. E. Cahill and R. J. Glauber, Density operators for fermions, *Physical Review A* **59**, 1538 (1999).
  - [11] S. Szalay, Z. Zimborás, M. Máté, G. Barcza, C. Schilling, and Ö. Legeza, Fermionic systems for quantum information people, *Journal of Physics A: Mathematical and Theoretical* **54**, 393001 (2021).
  - [12] X. Lyu and K. Bu, Fermionic gaussian testing and non-gaussian measures via convolution, *arXiv preprint arXiv:2409.08180* (2024).
  - [13] E. Knill, Fermionic linear optics and matchgates, *arXiv preprint quant-ph/0108033* (2001).
  - [14] S. Bravyi, Classical capacity of fermionic product channels, *arXiv preprint quant-ph/0507282* (2005).
  - [15] M. Hebenstreit, R. Jozsa, B. Kraus, S. Strelchuk, and M. Yoganathan, All pure fermionic non-gaussian states are magic states for matchgate computations, *Phys. Rev. Lett.* **123**, 080503 (2019).
  - [16] Computational power of matchgates with supplementary resources, *Physical Review A* **102**, 052604 (2020).
  - [17] B. Dias and R. Koenig, Classical simulation of non-gaussian fermionic circuits (2023), *arXiv preprint arXiv:2307.12912*.
  - [18] J. Cudby and S. Strelchuk, Gaussian decomposition of magic states for matchgate computations, *arXiv preprint arXiv:2307.12654* (2023).
  - [19] O. Reardon-Smith, M. Oszmaniec, and K. Korzekwa, Improved simulation of quantum circuits dominated by free fermionic operations, *arXiv preprint arXiv:2307.12702* (2023).
  - [20] B. Dias and R. Koenig, Classical simulation of non-gaussian fermionic circuits, *Quantum* **8**, 1350 (2024).
  - [21] E. Bianchi, L. Hackl, and M. Kieburg, Page curve for fermionic gaussian states, *Physical Review B* **103**, L241118 (2021).
  - [22] P. Jordan and E. P. Wigner, *Über das paulische äquivalenzverbot* (Springer, 1993).
  - [23] R. Jozsa and A. Miyake, Matchgates and classical simulation of quantum circuits, *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences* **464**, 3089 (2008).
  - [24] D. J. Brod, Efficient classical simulation of matchgate circuits with generalized inputs and measurements, *Phys. Rev. A* **93**, 062332 (2016).
  - [25] D. P. DiVincenzo and B. M. Terhal, Fermionic linear optics revisited, *Found. Phys.* **35**, 1967 (2004).
  - [26] B. Zumino, Normal forms of complex matrices, *Journal of Mathematical Physics* **3**, 1055 (1962).
  - [27] D. K. Hoffman, R. C. Raffanetti, and K. Ruedenberg, Generalization of euler angles to n-dimensional orthogonal matrices, *Journal of Mathematical Physics* **13**, 528 (1972).
  - [28] S. B. Bravyi and A. Y. Kitaev, Fermionic quantum computation, *Annals of Physics* **298**, 210 (2002).
  - [29] P.-O. Löwdin, Quantum theory of many-particle systems. ii. study of the ordinary hartree-fock approximation, *Physical Review* **97**, 1490 (1955).
  - [30] R. Wille, R. Van Meter, and Y. Naveh, Ibm’s qiskit tool chain: Working with and developing for real quantum computers, in *2019 Design, Automation & Test in Europe Conference & Exhibition (DATE)* (IEEE, 2019) pp. 1234–1240.

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### Appendix A: Lie theory of Fermionic Gaussian operators

The Clifford algebra  $\mathcal{C}_{2n}$  forms a Lie algebra under the commutator bracket  $[\gamma_J, \gamma_K]$ . In this section, we examine the subalgebras related to Gaussian and displaced Gaussian unitaries, originally defined in [13]. These constructions are foundational, as they support many of the later results and proofs presented in this work.

**Definition A.1** (Gaussian Lie algebras and groups). *Let  $\mathfrak{dg}(n)$  denote the Lie algebra of quadratic polynomials*

$$\mathfrak{dg}(n) = \{a\gamma_j + b\gamma_k\gamma_l \in \mathcal{C}_{2n} \mid \{a, b\} \subset \mathbb{C}, \{j, k, l\} \subset [2n]\}, \quad \dim \mathfrak{dg}(n) = 2n^2 + n. \quad (\text{A.1})$$

*Let  $\mathfrak{g}(n) \subsetneq \mathfrak{dg}(n)$  denote the Lie subalgebra of  $\mathfrak{dg}(n)$  of quadratic monomials, with dimension  $2n^2 - n$ :*

$$\mathfrak{g}(n) = \{a\gamma_j\gamma_k \mid a \in \mathbb{C}, \{j, k\} \subset [2n], j \neq k\}. \quad (\text{A.2})$$

*The image of  $\mathfrak{g}(n), \mathfrak{dg}(n)$  under the exponential map are the group  $G(n)$  of even Gaussian unitaries and  $DG(n) \supsetneq G(n)$  of displaced Gaussian unitaries, respectively.*

The following isomorphism can be verified by direct computation of the Lie bracket.

**Proposition A.1** (even Gaussian algebra isomorphism). *The even Gaussian Lie algebra  $\mathfrak{g}(n)$  is isomorphic to the algebra of antisymmetric matrices  $\mathfrak{so}(2n)$  under  $\varphi : \mathfrak{g}(n) \rightarrow \mathfrak{so}(2n)$  defined by:*

$$\varphi(\gamma_a\gamma_b) = 2s_{ab}, \quad s_{ab} = |a\rangle\langle b| - |b\rangle\langle a|, \quad a \neq b. \quad (\text{A.3})$$

An embedding is an injective homomorphism of algebras. The next embedding introduced in [13] is central to the constructions we use in this work.

**Definition A.2** (Clifford algebra embedding). *The following map  $\phi : \mathcal{C}_{2n} \rightarrow \mathcal{C}_{2n+1}$  is an embedding of the Clifford algebra, extended multiplicatively from the generators according to*

$$\phi(\gamma_j) = i\gamma_j\gamma_{2n+1}. \quad (\text{A.4})$$

*For an arbitrary basis element  $\gamma_J \in \mathcal{C}_{2n}$  of degree  $|J| = m$ , we obtain*

$$\phi(\gamma_J) = \begin{cases} i\gamma_J\gamma_{2n+1} & m \text{ odd}, \\ \gamma_J & m \text{ even} \end{cases}. \quad (\text{A.5})$$

Since  $\phi$  acts as an injective homomorphism by extending multiplicatively from its action on generators, it respects the Lie bracket. Consequently,  $\phi$ , when restricted to  $\mathfrak{dg}(n)$ , provides a Lie algebra embedding  $\mathfrak{dg}(n) \rightarrow \mathfrak{g}(n+1)$ . Composing  $\varphi$  and  $\phi$  yields the raw extended covariance matrix (equation II.7), and the following property explains the ubiquity of the extended covariance matrix in the theory of displaced Gaussian operators.

**Proposition A.2** ( $\mathfrak{dg}(n)$  to  $\mathfrak{so}(2n+1)$  embedding). *The composition  $2\bar{\Sigma} = \varphi \circ \phi : \mathfrak{dg}(n) \rightarrow \mathfrak{so}(2n+1)$  satisfying*

$$O = \frac{1}{2}\gamma^T M \gamma + d^T \gamma \in \mathfrak{dg}(n) \implies 2\bar{\Sigma}(O) = 2 \begin{bmatrix} M & id \\ -id^T & 0 \end{bmatrix} \in \mathfrak{so}(2n+1, \mathbb{C}) \quad (\text{A.6})$$

*is an isomorphism between the antisymmetric Lie algebra and the displaced Gaussian algebra.*

Observe that the quadratic terms  $2\bar{\Sigma}(\gamma_j\gamma_k) = 2s_{jk}$ , where  $1 \leq j < k \leq 2n$ , generate rotations between the  $j, k$ -th subspaces, while the linear terms  $2\bar{\Sigma}(\gamma_j) = 2is_{j(2n+1)}$  induce rotations between the  $j$ -th and  $(2n+1)$ -th subspaces.

## Appendix B: Wick's formula

**Definition B.1** (Pfaffian). *Given an antisymmetric matrix  $M \in \mathfrak{so}(2n, \mathbb{C})$ , the Pfaffian of  $M$  is defined by*

$$\text{Pf}(M) = \frac{1}{2^n n!} \sum_{\sigma \in S_{2n}} \prod_{l=1}^n M_{\sigma(2l-1), \sigma(2l)}. \quad (\text{B.1})$$

*Given an even multi-index  $J \subset [n]$  with  $|J| = 2m$ , we denote by  $M_{|J} \subset \mathfrak{so}(|J|, \mathbb{C})$  the restriction of  $M$  to the subspaces indexed by  $J$ . The component formula and Pfaffian are, correspondingly*

$$(M_{|J})_{jk} = M_{J_j J_k} \implies \text{Pf}(M_{|J}) = \frac{1}{2^m m!} \sum_{\sigma \in S_{2m}} \prod_{l=1}^m M_{J_{\sigma(2l-1)} J_{\sigma(2l)}}. \quad (\text{B.2})$$

A displaced Gaussian state is completely specified by its extended covariance. The following result slightly generalizes Wick's formula for even Gaussian states [2] to the nonzero-mean case. It is the anti-commuting counterpart of the classical Isserlis-Wick theorem for computing the higher-order moments of multivariate Gaussian distributions.

**Proposition B.1** (restatement of proposition III.1). *The  $J$ th moment of a displaced Gaussian state  $\rho$ , is expressible in terms of  $\tilde{\Sigma}(\rho)$  using the following formula:*

$$\rho_J = \alpha_{|J|} \text{Pf} \left[ \tilde{\Sigma}(\rho)_{|\tilde{J}} \right], \quad \tilde{J} = \begin{cases} J & |J| \text{ even} \\ J \cup \{2n+1\} & |J| \text{ odd} \end{cases}, \quad \alpha_{|J|} = (-i)^{|J| \bmod 2} \quad (\text{B.3})$$

Here  $\tilde{\Sigma}(\rho)_{|\tilde{J}}$  denotes the restriction of  $\tilde{\Sigma}(\rho)$  to the subspaces indexed by  $\tilde{J}$  as in equation B.2. Equivalently,

$$\rho = \frac{1}{2^n} \sum_J \rho_J \gamma_J = \frac{1}{2^n} \sum_J \alpha_{|J|} \text{Pf} \left[ \tilde{\Sigma}(\rho)_{|\tilde{J}} \right] \gamma_J. \quad (\text{B.4})$$

*Proof.* We begin by denoting the covariance and mean vectors as  $\Sigma = \Sigma(\rho)$  and  $\mu = \mu(\rho)$ , respectively. Expanding the Fourier transform definition, we have:

$$\begin{aligned} \Xi_\rho(\theta) &= \sum_J \rho_J \theta_J = \sum_{k=1}^{2n} \frac{1}{k!} \left( \frac{1}{2} \theta^T \Sigma \theta + \mu^T \theta \right)^k \\ &= \sum_{k=1}^n \frac{1}{k!} \left[ \left( \frac{1}{2} \theta^T \Sigma \theta \right)^k + k \left( \frac{1}{2} \theta^T \Sigma \theta \right)^{k-1} (\mu^T \theta) \right]. \end{aligned} \quad (\text{B.5})$$

This last equality holds because only two terms in the binomial expansion of each  $k$ -th power are non-zero. In particular, any term containing more than one factor of  $(\mu^T \theta)$  vanishes since  $(\mu^T \theta)^2 = 0$ . Hence, we obtain:

$$\left( \frac{1}{2} \theta^T \Sigma \theta + \mu^T \theta \right)^k = \left( \frac{1}{2} \theta^T \Sigma \theta \right)^k + k \left( \frac{1}{2} \theta^T \Sigma \theta \right)^{k-1} (\mu^T \theta). \quad (\text{B.6})$$

Now, consider the case where  $|J| = 2m$  (i.e.,  $J$  has even degree). According to equation B.5, the coefficient  $\rho_J$  is found as the term in front of  $\theta_J$  in the expansion:

$$\begin{aligned} \frac{1}{2^m m!} \left( \sum_{j,k=1}^{2n} \Sigma_{jk} \theta_j \theta_k \right)^m &= \sum_{|K|=2m} \frac{1}{2^m m!} \sum_{\sigma \in S_{2m}} \prod_{l=1}^m \Sigma_{K_{\sigma(2l-1)} K_{\sigma(2l)}} \theta_K \\ &= \sum_{|K|=2m} \text{Pf}(\Sigma_{|K}) \theta_K = \sum_{|K|=2m} \text{Pf} \left[ \tilde{\Sigma}(\rho)_{|K} \right] \theta_K. \end{aligned}$$

Here, the first equality follows from the combinatorics, the second from equation B.2, and the final line follows by applying equation B.3, noting that the sum is over multi-indices  $K \subset [2n]$  of size  $|J| = 2m$ . This completes the proof for even-degree  $J$ . For odd  $|J| = 2m - 1$ , we focus on the odd term in equation B.5, which expands to  $\frac{1}{(m-1)!} \left( \frac{1}{2} \theta^T \Sigma \theta \right)^{m-1} (\mu^T \theta)$ . Here,  $\rho_J$  corresponds to the term in front of  $\theta_J$  in this expansion. Since  $\mu^T \theta$  is the sole odd



term in this product, it commutes with every other term. This justifies the introduction of an additional Grassmann variable. Writing  $\tilde{\theta} = (\theta_1, \dots, \theta_{2n}, \theta_{2n+1})$ ,  $\rho_J$  corresponds to the coefficient of  $\theta_J$  in:

$$\begin{aligned} \frac{1}{(m-1)!} \left( \frac{1}{2} \theta^T \Sigma \theta \right)^{m-1} (\mu^T \theta) &\mapsto \frac{1}{(m-1)!} \left( \frac{1}{2} \tilde{\theta}^T \begin{bmatrix} \Sigma & 0_{2n \times 1} \\ 0_{1 \times 2n} & 0 \end{bmatrix} \tilde{\theta} \right)^{m-1} \left( \frac{1}{2} \theta^T \mu \cdot \theta_{2n+1} - \frac{1}{2} \theta_{2n+1} \cdot \mu^T \theta \right) \\ &= (-i) \frac{1}{(m-1)!} \left( \frac{1}{2} \tilde{\theta}^T \begin{bmatrix} \Sigma & 0_{2n \times 1} \\ 0_{1 \times 2n} & 0 \end{bmatrix} \tilde{\theta} \right)^{m-1} \left( \frac{1}{2} \tilde{\theta}^T \begin{bmatrix} 0_{2n \times 2n} & i\mu \\ -i\mu^T & 0 \end{bmatrix} \tilde{\theta} \right) \\ &= (-i) \sum_{|K|=2m, 2n+1 \in K} \text{Pf} \left[ \tilde{\Sigma}(\rho)_{|K} \right] \tilde{\theta}_K. \end{aligned}$$

This completes the proof that for odd-degree  $J$  that  $\rho_J = (-i) \text{Pf} \left[ \tilde{\Sigma}(\rho)_{|J} \right]$ .  $\square$

### Appendix C: Conjugate action of $DG(n)$

The first step in understanding displaced Gaussian operators is characterizing the conjugate action of  $DG(n)$ . We begin by identifying this conjugate action on  $\mathfrak{dg}(n) \subset \mathcal{C}_{2n}$ , which turns out to be a rotation of the quadratic polynomials. We next show that this property tensorizes properly, yielding a compact form for conjugation on  $\mathcal{C}_{2n}$ . Finally, we derive the conjugate action of displaced Gaussian unitaries on displaced Gaussian states.

**Lemma C.1** (displaced Gaussian action on  $\mathfrak{dg}(n)$ ). *Given  $O \in \mathfrak{dg}(n)$  and displaced Gaussian unitary  $U \in DG(n)$*

$$O = \frac{1}{2} \gamma^T M \gamma + v^T \gamma, \quad U = e^B, \quad B = \frac{1}{2} \gamma^T h \gamma + id^T \gamma \in \mathfrak{dg}(N). \quad (\text{C.1})$$

The conjugate action of  $U$  on  $O$  satisfies, for  $\log U = B \in \mathfrak{dg}(n)$ ,

$$\tilde{\Sigma}(UOU^\dagger) = R \tilde{\Sigma}(O) R^T, \quad R = e^{2\tilde{\Sigma}(\log U)}. \quad (\text{C.2})$$

We can expand the definitions to obtain the explicit formula:

$$UOU^\dagger = \frac{1}{2} \gamma^T A \gamma + u^T \gamma \quad \text{where} \quad \begin{bmatrix} A & iu \\ -iu^T & 0 \end{bmatrix} = R \begin{bmatrix} M & iv \\ -iv^T & 0 \end{bmatrix} R^T, \quad R = \exp \left( 2 \begin{bmatrix} h & -d \\ d^T & 0 \end{bmatrix} \right). \quad (\text{C.3})$$

Setting  $M = 0$  and  $d = 0$  specializes to the known action of even Gaussian unitaries ([23, Theorem 3]).

*Proof.* Using the Baker-Campbell-Hausdorff formula, conjugation is determined by the Lie bracket on  $\mathfrak{dg}_n$ :

$$\begin{aligned} UOU^\dagger &= e^B O e^{-B} = O + [B, O] + \frac{1}{2!} [B, [B, O]] + \frac{1}{3!} [B, [B, [B, O]]] + \dots \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \text{ad}_B^n(O), \quad \text{ad}_B(O) = [B, O]. \end{aligned}$$

Using the compatibility of the adjoint map with  $2\tilde{\Sigma}$  (proposition A.2) yields

$$2\tilde{\Sigma}(UOU^\dagger) = \sum_{n=0}^{\infty} \frac{1}{n!} \text{ad}_{2\tilde{\Sigma}(B)}^n [2\tilde{\Sigma}(O)] = e^{2\tilde{\Sigma}(B)} 2\tilde{\Sigma}(O) e^{-2\tilde{\Sigma}(B)}. \quad (\text{C.4})$$

$\square$

**Lemma C.2.** *Given  $U = \exp(\gamma^T h \gamma / 2) \in G(n)$ , its conjugate action affects a Majorana basis element  $\gamma_J$  by antisymmetrized rotation within the degree- $m$  subspace:*

$$U \gamma_J U^\dagger = \sum_{|K|=|J|} R_{\hat{K}, J} \gamma_K, \quad R = e^{2h}. \quad (\text{C.5})$$

Here the sum is over all size- $m$  multi-indices (sorted subsets of  $[2n]$ ), and  $R_{\hat{K}, J}$  denotes the following antisymmetrized product defined for  $|J| = |K| = m$  (for example,  $R_{\widehat{[a,b]}, [c,d]} = R_{ac} R_{bd} - R_{bc} R_{ad}$ ):

$$R_{\hat{K}, J} = \sum_{\sigma \in S_m} \text{sgn}(\sigma) \prod_{i=1}^{|J|} R_{K_{\sigma(i)}, J_i}. \quad (\text{C.6})$$

*Proof.* Substituting  $M, d = 0$  in lemma C.1 shows that  $U \in G(n)$  affects a rotation of the generators:

$$U\gamma_j U^\dagger = \sum_{k=1}^{2n} R_{kj} \gamma_k, \quad R = e^{2h}, \quad \forall j \in [2n]. \quad (\text{C.7})$$

To see how equation C.7 implies C.5, expand

$$\begin{aligned} U\gamma_J U^\dagger &= \prod_{j=1}^m U\gamma_{J_j} U^\dagger = \prod_{j=1}^m \left( \sum_{k=1}^{2n} R_{k,J_j} \gamma_k \right) \\ &= \left( \sum_{K_1=1}^{2n} R_{K_1,J_1} \gamma_{K_1} \right) \cdots \left( \sum_{K_m=1}^{2n} R_{K_m,J_m} \gamma_{K_m} \right) \\ &= \sum_{K_1=1}^{2n} \cdots \sum_{K_m=1}^{2n} \left( \prod_{i=1}^m R_{K_i,J_i} \right) \gamma_K = \sum_{|K|=m} R_{\hat{K},J} \gamma_K. \end{aligned}$$

In the last equality, the  $(K_1, \dots, K_m)$  cannot contain duplicates due to the orthogonality of  $R$  and the elements of  $J$  being distinct: it is insightful to investigate the  $m = 2$  case, in which case the duplicate terms sum to

$$\sum_{k=1}^{2n} R_{k,J_1} R_{k,J_2} \gamma_k^2 = 2I(R^T R)_{J_1,J_2} = 0.$$

Consequently, the sum over distinct  $(K_1, \dots, K_m)$  can be decomposed into a sum over sorted  $(K_1, \dots, K_m)$  together with a sum over all permutations over  $S_m$ , yielding the desired equation.  $\square$

We are now ready to prove the conjugate action of  $DG(n)$  on all of  $\mathcal{C}_{2n}$ . Recall the definition of  $\tilde{J}$  in B.1 and the antisymmetrized product  $R_{\tilde{L},J}$  in equation C.6. The following result shows that conjugating  $\gamma_J$  by  $U$  is equivalent to adjoining an additional  $\gamma_{2n+1}$  using  $\phi$ , rotating the even basis  $\gamma_{\tilde{J}}$  using the antisymmetrized  $R$  as in equation C.6, then deleting the adjoined mode.

**Theorem C.3** (displaced Gaussian action on  $\mathcal{C}_{2n}$ ). *Given  $U \in DG(n) \subset \mathcal{C}_{2n}$  effecting  $R \in SO(2n+1)$  per lemma C.1. its conjugate action affects a Majorana monomial  $\gamma_J \in \mathcal{C}_{2n}$  by the following equation:*

$$U\gamma_J U^\dagger = \sum_{|\tilde{K}|=|\tilde{J}|} R_{\hat{\tilde{K}},\tilde{J}} \gamma_{\tilde{K}} \quad (\text{C.8})$$

where the sum is over all multi-indices  $K \subset [2n]$  such that  $|\tilde{K}| = |\tilde{J}|$ .

*Proof.* Recall equation A.5 and let  $\phi(\gamma_J) = \alpha_{|J|} \gamma_{\tilde{J}}$ , where  $\alpha_{|J|} = i^{|J| \bmod 2}$ . Let  $U = e^B \in DG(n)$  with  $B$  quadratic and  $\tilde{U} = \phi(e^B) = e^{\phi(B)} \in G(n+1)$ , we obtain

$$\phi(U\gamma_J U^\dagger) = \phi \left[ \sum_{n=0}^{\infty} \frac{1}{n!} \text{ad}_B^n(\gamma_J) \right] = \sum_{n=0}^{\infty} \frac{1}{n!} \text{ad}_{\phi(B)}^n[\phi(\gamma_J)] = e^{\phi(B)} \phi(\gamma_J) e^{-\phi(B)} = \alpha_{|J|} \tilde{U} \gamma_{\tilde{J}} \tilde{U}^\dagger.$$

Let  $R = e^{2\tilde{\Sigma}(\log U)} \in SO(2n+1)$  be the rotation corresponding to  $U$  in lemma C.1, and  $\tilde{R} \in SO(2n+2)$  be the rotation corresponding to the even Gaussian unitary  $\tilde{U}$ . They are related by

$$\tilde{R} = \exp \left( 2 \begin{bmatrix} h & -d \\ d^T & 0 \end{bmatrix} \oplus (0) \right) = R \oplus (1) \in SO(2n+2). \quad (\text{C.9})$$

Invoking lemma C.2 on the even conjugate action  $\tilde{U}\gamma_{\tilde{J}}\tilde{U}^\dagger$  yields

$$\phi(U\gamma_J U^\dagger) = \alpha_{|J|} \tilde{U} \gamma_{\tilde{J}} \tilde{U}^\dagger = \alpha_{|J|} \sum_{|\tilde{K}|=|\tilde{J}|, \tilde{K} \subset [2n+2]} \tilde{R}_{\hat{\tilde{K}},\tilde{J}} \gamma_{\tilde{K}} = \alpha_{|J|} \sum_{|\tilde{K}|=|\tilde{J}|, \tilde{K} \subset [2n+1]} R_{\hat{\tilde{K}},\tilde{J}} \gamma_{\tilde{K}}$$

The last equality holds in light of equation C.9: we can ignore the  $(2n+2)$ -th subspace since the conjugated term  $\phi(\gamma_J)$  does not contain  $\gamma_{2n+2}$  and  $\tilde{R}$  acts trivially on this subspace. Noting that  $\alpha_{|J|} = \alpha_{|K|}$  for  $|\tilde{K}| = |\tilde{J}|$  (since  $\alpha_J$  only depends on the degree), apply  $\phi^{-1}$  to both sides yields the desired relation.  $\square$

To analyze how a displaced Gaussian unitary acts on Gaussian states, we need a lemma concerning the Pfaffian.

**Lemma C.4.** *Given an antisymmetric covariance matrix  $A \in \mathfrak{so}(2n, \mathbb{C})$  and a rotation matrix  $R \in SO(2n, \mathbb{R})$ , the following equation holds for all  $m = 1, \dots, n$ :*

$$\sum_{|K|=|J|=2m} \text{Pf}(A_{|J}) R_{\hat{K},J} \gamma_K = \sum_{|J|=2m} \text{Pf}[(RAR^T)_{|J}] \gamma_J \quad (\text{C.10})$$

with  $R_{\hat{K},J}$  as defined in equation C.6; the left-hand sum is over even multi-indices  $J, K \subset [2n]$  with  $|J| = |K| = 2m$ .

*Proof.* It is known that ([23], Theorem 3), given an even Gaussian state  $\rho$  and  $U = e^B \in G(n)$ , the state  $U\rho U^\dagger$  remains even Gaussian and has the following covariance matrix:

$$\Sigma(U\rho U^\dagger) = R\Sigma(\rho)R^T, \quad R = e^{2\bar{\Sigma}(B)}.$$

Let  $A = \Sigma(\rho)$ , apply Wick's formula B.1 to  $U\rho U^\dagger$  to obtain the right-hand side of equation C.10:

$$U\rho U^\dagger = \frac{1}{2^n} \sum_J \text{Pf}[\Sigma(U\rho U^\dagger)_{|J}] \gamma_J = \frac{1}{2^n} \sum_J \text{Pf}[(RAR^T)_{|J}] \gamma_J.$$

To obtain the left-hand side in equation C.10, apply lemma C.2 to each term in the Wick's formula expansion of  $\rho$ :

$$U\rho U^\dagger = \frac{1}{2^n} \sum_J \text{Pf}(A_{|J}) U \gamma_J U^\dagger = \frac{1}{2^n} \sum_J \text{Pf}(A_{|J}) \sum_{|K|=|J|} R_{\hat{K},J} \gamma_K.$$

To conclude the proof, the two expressions for  $U\rho U^\dagger$  implies the following equation, which must also hold for each degree  $|J| = |K| = 2m$  separately since addition does not change the degree of a term:

$$\sum_J \text{Pf}[(RAR^T)_{|J}] \gamma_J = \sum_J \text{Pf}(A_{|J}) \sum_{|K|=|J|} R_{\hat{K},J} \gamma_K.$$

□

**Theorem C.5** (restatement of theorem III.2). *Applying a displaced Gaussian unitary  $U \in G(n)$  to  $\rho \in \mathbf{DGauss}(n)$  results in a displaced Gaussian state with the extended covariance matrix*

$$\tilde{\Sigma}(U\rho U^\dagger) = R\tilde{\Sigma}(\rho)R^T \text{ where } R = e^{2\bar{\Sigma}(\log U)}. \quad (\text{C.11})$$

Here  $\log U \in \mathfrak{dg}(n)$  is proportional to the quadratic Hamiltonian generating  $U$ , and  $\bar{\Sigma}$  is defined in equation II.7.

*Proof.* The first equality below follows from applying Wick's formula B.1 to  $U\rho U^\dagger$ . It remains to demonstrate the second inequality in

$$\frac{1}{2^n} \sum_{J \subset [2n]} \alpha_J \text{Pf}[\tilde{\Sigma}(U\rho U^\dagger)_{|J}] \gamma_J = U\rho U^\dagger = \frac{1}{2^n} \sum_{J \subset [2n]} \alpha_J \text{Pf}[(R\tilde{\Sigma}(\rho)R^T)_{|J}] \gamma_J.$$

To do so, apply theorem C.3 to each term in the Wick expansion of  $\rho$  to obtain

$$U\rho U^\dagger = \frac{1}{2^n} \sum_J \alpha_J \text{Pf}[\Sigma(\rho)_{\tilde{J}}] U \gamma_J U^\dagger = \frac{1}{2^n} \sum_J \alpha_J \text{Pf}[\Sigma(\rho)_{\tilde{J}}] \sum_{|\hat{K}|=|\tilde{J}|} R_{\hat{K},\tilde{J}} \gamma_K.$$

Noting that  $\alpha_J$  only depends on  $|J|$ , invoking lemma C.4 with  $(\tilde{J}, \hat{K})$  in place of  $(J, K)$  concludes the proof:

$$U\rho U^\dagger = \frac{1}{2^n} \sum_J \sum_{|\hat{K}|=|\tilde{J}|} \alpha_J \text{Pf}[\Sigma(\rho)_{\tilde{J}}] R_{\hat{K},\tilde{J}} \gamma_K = \frac{1}{2^n} \sum_J \alpha_J \text{Pf}[(R\Sigma(\rho)R^T)_{|J}] \gamma_J.$$

□

## Appendix D: Characterization of displaced Gaussian states

In this section, we unify three reasonable definitions of displaced Gaussian states and show that they are equivalent. This is done by first establishing this characterization for a special diagonalizable subclass of displaced Gaussian states, then extending this result by showing that the full set of displaced Gaussian states is the orbit of the diagonalizable Gaussian states under  $DG(n)$ .

**Definition D.1** (diagonalized Gaussian states). *A displaced Gaussian state  $\rho_D \in \mathcal{C}_{2n}$  is a diagonalized Gaussian state if its extended covariance matrix is block-diagonalized:*

$$\tilde{\Sigma}(\rho_D) = i \left( \bigoplus_{j=1}^n \begin{bmatrix} 0 & \lambda_j \\ -\lambda_j & 0 \end{bmatrix} \right) \oplus (0) \in \mathfrak{so}(2n+1, \mathbb{C}).$$

**Lemma D.1** (diagonalizable Gaussians are separable computational basis mixtures). *With  $\lambda_1$  as in definition D.1:*

$$\rho_D = \bigotimes_{j=1}^n \left( \frac{1+\lambda_j}{2} |0\rangle\langle 0| + \frac{1-\lambda_j}{2} |1\rangle\langle 1| \right).$$

*Proof.* Expand the Grassmann expression of  $\rho_D(\theta)$  using the covariance matrix:

$$\rho_D(\theta) = \exp \left[ \frac{1}{2} \theta^T \Sigma(\rho_D) \theta \right] = \exp \left( \sum_{j=1}^n \lambda_j \theta_{2j-1} \theta_{2j} \right) = \bigotimes_{j=1}^n \exp(i \lambda_j \theta_1 \theta_2) = \bigotimes_{j=1}^n 1 + i \lambda_j \theta_1 \theta_2 \quad (\text{D.1})$$

Replacing  $\theta_j \mapsto \gamma_j$  and recognizing  $i \gamma_1 \gamma_2 = Z$  yields the desired equation

$$\rho_D = \frac{1}{2^n} \bigotimes_{j=1}^n 1 + i \lambda_j \gamma_1 \gamma_2 = \bigotimes_{j=1}^n \frac{1 + i \lambda_j \gamma_1 \gamma_2}{2} = \bigotimes_{j=1}^n \frac{1 + \lambda_j Z}{2} = \bigotimes_{j=1}^n \left( \frac{1+\lambda_j}{2} |0\rangle\langle 0| + \frac{1-\lambda_j}{2} |1\rangle\langle 1| \right) \quad (\text{D.2})$$

□

**Lemma D.2** (diagonalizable Gaussian states as thermal states). *Every diagonalizable Gaussian state  $\rho_D \in \mathcal{C}_{2n}$  as in definition D.1 is the thermal (ground) state of a quadratic Hamiltonian  $H \in \mathfrak{g}(n)$ :*

$$\rho_D = \frac{e^H}{\text{Tr}(e^H)}, \quad H = \frac{i}{2} \gamma^T h \gamma, \quad h = \bigoplus_{j=1}^n \begin{bmatrix} 0 & \tanh^{-1} \lambda_j \\ -\tanh^{-1} \lambda_j & 0 \end{bmatrix} \quad (\text{D.3})$$

*Proof.* Using lemma D.1: w.l.o.g. we can consider a single-qubit with  $h_1 = \arctan(\lambda_1)(|0\rangle\langle 1| - |1\rangle\langle 0|)$ , then

$$H_1 = \frac{i}{2} \begin{pmatrix} \gamma_1 \\ \gamma_2 \end{pmatrix}^T \begin{pmatrix} 0 & \tanh^{-1} \lambda \\ -\tanh^{-1} \lambda & 0 \end{pmatrix} \begin{pmatrix} \gamma_1 \\ \gamma_2 \end{pmatrix} = (\tanh^{-1} \lambda) Z$$

The thermal state of  $H_1$  is  $\frac{1}{2} [(1+\lambda)|0\rangle\langle 0| + (1-\lambda)|1\rangle\langle 1|]$ . Pure states with  $\lambda = \pm 1$  are defined as the limit. □

**Lemma D.3** (diagonalizability of displaced Gaussian states). *For every displaced Gaussian state  $\rho \in \mathcal{C}_{2n}$ , there exists  $U \in DG(n)$  such that  $U \rho U^\dagger$  is a diagonalized Gaussian state. If  $\rho$  is an even Gaussian state, then  $U$  will be even.*

*Proof.* By standard matrix theory [26], for every  $A \in \mathfrak{so}(m, \mathbb{R})$  there exists a rotation  $R \in SO(m, \mathbb{R})$  such that  $R A R^T$  is block-diagonal. lemma C.1 shows that the displaced Gaussian unitaries  $DG(n) \cong SO(2n+1)$  and that rotations acting trivially on the last subspace are generated by the even Gaussian unitaries. Given a displaced Gaussian state  $\rho$ ,  $\tilde{\Sigma}(\rho)$  is antisymmetric thus block-diagonalizable by the conjugate action of some  $U \in DG(n)$  per theorem C.5. If  $\rho$  is even,  $\tilde{\Sigma}(\rho)$  is trivial on the last subspace thus block-diagonalizable by  $U \in G(n)$ . □

**Theorem D.4** (restatement of theorem III.3). *A  $n$ -qubit state  $\rho \in \mathbf{DGauss}(n)$  iff any of the following holds:*

1. Thermal state definition:  $\rho$  is the thermal state of some quadratic Hamiltonian  $H \in \mathfrak{dg}(n)$ ,

$$\rho = \frac{e^H}{\text{Tr}(e^H)}, \quad H = \frac{i}{2} \gamma^T h \gamma + d^T \gamma. \quad (\text{D.4})$$

*If  $\rho$  is pure, then  $\rho$  is the ground state of some quadratic Hamiltonian.*

2. Circuit definition:  $\rho$  is the result of a displaced Gaussian unitary acting on a separable computational basis state:

$$\rho = U_G \rho_D U_G^\dagger, \quad U_G \in DG(n), \quad \rho_D \text{ diagonal Gaussian.} \quad (\text{D.5})$$

3. Fourier definition: The Fourier transform of  $\rho$  admits a Gaussian expression:

$$\Xi_\rho(\theta) = \exp\left(\frac{i}{2}\theta^T M \theta + d^T \theta\right) \quad (\text{D.6})$$

*Proof.* (3  $\implies$  1 and 2): given  $\rho \in \mathcal{C}_{2n}$  with a Gaussian Fourier expression, lemma D.3 provides  $U_G \in DG(n)$  such that  $U\rho U^\dagger = \rho_D$  is a diagonalized Gaussian state, from which (2) immediately follows. lemma D.2 implies that  $\rho_D \propto e^{H_D}$  for some quadratic  $H_D$ , thus  $\rho = U^\dagger \rho_D U \propto e^{U_G^\dagger H_D U_G}$  is the thermal state of the Hamiltonian  $U_G^\dagger H_D U_G$  which remains quadratic by lemma C.1. The implication (2  $\implies$  3) follows from theorem C.5, and (1  $\implies$  3) follows from block-diagonalizing  $\tilde{\Sigma}(H)$  using  $U_G$  such that  $U_G \rho U_G^\dagger = \rho_D$ , identifying the Fourier expression of  $\rho_D$ , then applying theorem C.5 to  $U_G^\dagger \rho_D U_G = \rho$ .  $\square$

## Appendix E: Classical simulation of displaced Gaussian circuits

It has been shown that every  $U \in G(n)$  has a decomposition into  $O(n^3)$  local n.n. matchgates which act on at most two consecutive lines [23, Theorem 5]. The following result extends this decomposition by applying the same technique slightly adopted to displaced Gaussian states.

**Theorem E.1** (restatement of theorem IV.1). *Every  $U \in DG(n)$  can be decomposed into the product of  $O(n^3)$  gates which are either matchgates or single-qubit gates on the initial line of the Jordan-Wigner transform.*

*Proof.* Proposition A.2 shows that  $DG(n) \cong SO(2n+1)$ . Examining the embedding equation for the rotation  $R$ ,

$$\log R = 2\tilde{\Sigma} \left( \frac{1}{2}\gamma^T C \gamma + d^T \gamma \right) = 2 \begin{bmatrix} C & id \\ -id^T & 0 \end{bmatrix},$$

we see that the quadratic forms  $\frac{1}{2}\gamma^T C \gamma$  generate rotations within the first  $2n$  subspaces. Single-qubit gates can be generated using  $R_z$  (a matchgate) along with  $R_x$ , where  $R_x(\theta) = \exp(i\theta X/2) = \exp(i\theta\gamma_1/2)$ , to create rotations between the first and  $(2n+1)$ -th subspaces under  $2\tilde{\Sigma}$ . An element of  $SO(2n+1)$  can be decomposed into  $O(n^2)$  rotations between pairs of subspaces via the method of Euler angles [27]. Further, each rotation between two arbitrary subspaces can be implemented with  $O(n)$  rotations between the  $(j, k)$ -th subspaces (for  $1 \leq j < k \leq 2n$ ) or between the first and  $(2n+1)$ -th subspaces. Thus, the total decomposition requires  $O(n^3)$  gates, each of which is either a matchgate or a single-qubit gate on the initial line of the Jordan-Wigner transform.  $\square$

The proposition below was essentially shown in Theorem 3 in [24].

**Proposition E.2** (restatement of proposition IV.2). *Every  $n$ -qubit product state is a displaced Gaussian state.*

*Proof.* We use the fermionic swap unitary first defined in [28]

$$S_{j \leftrightarrow k} = \exp \left[ \frac{\pi}{4} (\gamma_{2j-1} \gamma_{2k} - \gamma_{2j} \gamma_{2k-1} - \gamma_{2j-1} \gamma_{2j} - \gamma_{2k-1} \gamma_{2k}) \right] = S_{k \leftrightarrow j} = -S_{j \leftrightarrow k}^\dagger. \quad (\text{E.1})$$

The fermionic swap acts as a genuine swap if any one of the input lines is even. For every pure product state

$$|\psi\rangle = |\psi_1\rangle \cdots |\psi_n\rangle = (U_1 \otimes \cdots \otimes U_n) |0\rangle^{\otimes n}, \quad (\text{E.2})$$

we can implement it by computing  $U_n |0\rangle$  on the initial line, swapping it through the intermediate computational basis states to the  $n$ -th register, then do the same for  $U_{n-1} |0\rangle, \dots, U_1 |0\rangle$ . Since we're only using displaced Gaussian unitaries consisting of single-qubit states on the initial line and the fermionic swap, the resulting pure product state is a displaced Gaussian state; mixed product states follow by the same argument.  $\square$

Given a displaced Gaussian state input, the action of displaced Gaussian unitaries can be efficiently simulated by theorem C.5. We next consider the simulation of measurements in the computational basis, which can be done by computing the Grassmann integral of Gaussian operators. Using Gaussian integrals to facilitate simulation has been first considered in [4], and earlier treatments of such integrals can be found in [6, 29]. We first briefly recount the definition of the Grassmann integral and known results for Grassmann integrals.



**Definition E.1** (Grassmann differentiation and integration). *The partial derivative  $\partial_a : \mathcal{G}_n \rightarrow \mathcal{G}_n$  is the linear map*

$$\partial_a 1 = 0, \quad \partial_a \theta_b = \delta_{ab}. \quad (\text{E.3})$$

*Extended according to the Leibniz's rule  $\partial_a[\theta_b f(\theta)] = \delta_{ab} f(\theta) - \theta_b \partial_a f(\theta)$ . Integration is equivalent to differentiation*

$$\int d\theta_a \equiv \partial_a, \quad \int D\theta \equiv \int d\theta_n \cdots \int d\theta_2 \int d\theta_1. \quad (\text{E.4})$$

Formally,  $\partial_a$  acts on a monomial  $\theta_J$  by commuting  $\theta_a$  to the left (if it exists in  $\theta_J$ ), eliminating it, then keeping the remaining components; note that the image of  $\partial_a$  has no dependence on  $\theta_a$ . The order  $\int D\theta$  is chosen such that  $\int D\theta \theta_1 \cdots \theta_n = 1$ . Formally,  $\int D\theta$  extracts the complex coefficient before the highest-order monomial in the polynomial expansion of an operator. Given antisymmetric  $M \in \mathfrak{so}(2n, \mathbb{C})$ , we obtain ([4], equation 12):

$$\int D\eta \exp\left(\frac{1}{2}\eta^T M \eta\right) = \text{Pf}(M). \quad (\text{E.5})$$

Given a nonsingular antisymmetric matrix  $M \in \mathfrak{so}(2n, \mathbb{C})$  and two sets of Grassmann generators  $\{\eta_j\}_{j=1}^{2n}, \{\theta_j\}_{j=1}^{2n}$  which anticommute with each other, i.e.  $\{\theta_j, \eta_k\} = 0$ , then ([4], equation 13):

$$\int D\theta \exp\left(\eta^T \theta + \frac{1}{2}\theta^T M \theta\right) = \text{Pf}(M) \exp\left(\frac{1}{2}\eta^T M^{-1} \eta\right). \quad (\text{E.6})$$

Given  $X, Y \in \mathcal{C}_{2n}$  with Fourier transforms  $\Xi_X(\theta), \Xi_Y(\eta)$  where  $\theta, \mu$  are anti-commuting Grassmann generators, the trace of their product is ([4], equation 15):

$$\text{Tr}(XY) = \left(-\frac{1}{2}\right)^n \int D\eta D\theta e^{\eta^T \theta} \Xi_X(\eta) \Xi_Y(\theta). \quad (\text{E.7})$$

Using the formulas above, we obtain the following result which underpins the efficient simulation of measurements. Note that it crucially requires one of the inputs to be even.

**Lemma E.3** (Gaussian overlap formula). *Given a  $n$ -qubit displaced Gaussian state  $\rho$  and a  $n$ -qubit even Gaussian state  $\sigma$ , let  $A = \Sigma(\rho), B = \Sigma(\sigma)$ . If  $B$  is invertible, then*

$$\text{Tr}(\rho\sigma) = \frac{1}{2^n} \sqrt{\det(I + AB)}. \quad (\text{E.8})$$

*Proof.* Since  $\sigma$  is even, the overlap  $\text{Tr}(\rho\sigma)$  only depends on the even coefficients of  $\rho$ . Recalling Wick's formula B.1, the even coefficients of  $\rho$  are unchanged if we set the mean to zero. Thus without loss of generality expand

$$\Xi_\rho(\eta) = \exp\left(\frac{i}{2}\eta^T A \eta\right), \quad \Xi_\sigma(\theta) = \exp\left(\frac{i}{2}\theta^T B \theta\right).$$

First consider  $B$  invertible, using the trace equation E.7 and Gaussian integral equations E.5, E.6 yields

$$\begin{aligned} (-2)^n \text{Tr}(\rho\sigma) &= \int D\eta D\theta e^{\eta^T \theta} X(\eta) Y(\theta) \\ &= \int D\eta \exp\left(\frac{1}{2}\eta^T A \eta\right) \int D\theta e^{\eta^T \theta} \exp\left(\frac{1}{2}\theta^T B \theta\right) \\ &= \text{Pf}(B) \int D\eta \exp\left[\frac{1}{2}\eta^T (A + B^{-1}) \eta\right] = \text{Pf}(B) \text{Pf}(A + B^{-1}). \end{aligned}$$

Next note that  $\text{Pf}(A)^2 = \det A$  and that  $\text{Tr}(\rho\sigma)$  since  $\rho, \sigma$  are positive operators, then

$$4^n \text{Tr}(\rho\sigma)^2 = |\det(B) \det(A + B^{-1})| = |\det(AB + I)|.$$

Finally,  $AB$  is real since  $A, B$  are each purely imaginary matrices, and  $\det(AB + I)$  is positive since  $\|AB\| \leq \|A\| \|B\| \leq 1$  in the operator norm. This proves the result for invertible  $B$ . For the general case, let  $B_\epsilon = B + \epsilon I$  where  $\tilde{I} = \bigoplus_{j=1}^n |0\rangle\langle 1| - |1\rangle\langle 0|$  and  $\epsilon \ll 1$  and take  $\epsilon \rightarrow 0$ .  $\square$

**Lemma E.4** (restatement of lemma IV.3). *Given a  $n$ -qubit displaced Gaussian state  $\rho \in \mathcal{C}_{2n}$ , a subset  $K \subset [n]$  of lines to measure with  $|K| = k \leq n$ , and a computational basis  $x \in \{0, 1\}^k$  corresponding to the measurement operator*

$$O(K, x) = \frac{1}{2^k} \prod_{j=1}^k I + (-1)^{x_j} Z_{K_j}, \quad K \subset [2n], \quad x \in \{0, 1\}^k \quad (\text{E.9})$$

which is  $|x\rangle\langle x|$  when restricted to the lines indexed by  $K$ . The expectation value of the measurement is

$$\text{Tr}[O(K, x)\rho] = \frac{1}{2^k} \sqrt{\det[I + \Sigma(\rho)\Sigma(K, x)]}. \quad (\text{E.10})$$

Here  $\Sigma(K, x)$  is the antisymmetric covariance matrix associated with the measurement defined by

$$\Sigma(K, x) = -i \sum_{j=1}^k (-1)^{x_j} s_{(2K_j+1)(2K_j+2)} \in \mathfrak{so}(2n, \mathbb{C}), \quad s_{jk} = |j\rangle\langle k| - |k\rangle\langle j| \quad (\text{E.11})$$

*Proof.* Fixing  $K$  and  $x$ , let  $O = O(K, x)$ . Note that  $I/2$  is the maximally mixed state, so  $O = 2^{n-k} \rho_O$  where  $\rho_O = 2^{k-n} O \in \mathbf{DGauss}$ . The covariance matrix of  $\rho(O)$  is

$$\Sigma(\rho_O) = -i \sum_{j=1}^k (-1)^{x_j} s_{(2K_j+1)(2K_j+2)} = \Sigma(K, x).$$

Applying lemma E.3 concludes the proof since  $\text{Tr}[O(K, x)\rho] = 2^{n-k} \text{Tr}(\rho_O \rho) = 2^{n-k} \frac{1}{2^n} \sqrt{\det[I + \Sigma(\rho)\Sigma(K, x)]}$ .  $\square$

## Appendix F: Unitary embedding

In this section, begin by describing the first construction of a unitary embedding of  $n$ -qubit displaced Gaussian states into  $(n+1)$ -qubit even Gaussian states. Leveraging this tool, we generalize a previous work [12] on fermionic convolution and Gaussian testing to displaced Gaussian states. This yields useful operational protocols for testing efficiently simulable displaced Gaussian components as well as other characterizations of displaced Gaussian states.

**Definition F.1** (even embedding channel). *The even embedding channel  $\mathcal{E} : \mathcal{C}_{2n} \rightarrow \mathcal{C}_{2n+2}$  is defined by*

$$\mathcal{E}(\rho) = V(\rho \otimes |+\rangle\langle +|)V^\dagger \quad (\text{F.1})$$

where  $V \in \mathcal{C}_{2n+2}$  is the displaced Gaussian unitary defined by

$$V = \exp\left(-i\frac{\pi}{4}\gamma_{2n+2}\right). \quad (\text{F.2})$$

One can verify that  $V$  effects the following transform of the Majorana generators exactly as  $\phi$  in definition A.2:

$$V\gamma_j V^\dagger = \phi(\gamma_j) = \begin{cases} i\gamma_j \gamma_{2n+2} & j < 2n+2 \\ \gamma_{2n+2} & j = 2n+2 \end{cases}. \quad (\text{F.3})$$

To demonstrate that this is a desirable even embedding, we need the following lemma:

**Lemma F.1** (adjoining  $|+\rangle$  to an even Gaussian state). *Given an even Gaussian state  $\rho \in \mathbf{Gauss}(n)$  with  $M = \Sigma(\rho)$ , the product state  $\sigma = \rho \otimes |+\rangle\langle +|$  is a displaced Gaussian state with extended covariance*

$$\tilde{\Sigma}(\sigma) = \tilde{\Sigma}(\rho \otimes I/2) + i s_{(2n+1)(2n+3)} \in \mathfrak{so}(2n+3, \mathbb{C}), \quad s_{jk} = |j\rangle\langle k| - |k\rangle\langle j|. \quad (\text{F.4})$$

*Proof.* Define  $\tau = |+\rangle\langle +| \otimes \rho$ ; we obtain the expansion for  $\Xi_\tau$  as

$$\begin{aligned} \Xi_\tau(\theta) &= \Xi_{|+\rangle\langle +|}(\theta) \otimes \Xi_\rho(\theta) = \exp(\theta_1) \otimes \exp\left(\sum_{j < k=1}^{2n} M_{jk} \theta_j \theta_k\right) \\ &= \exp\left(\theta_1 + \sum_{j < k=1}^{2n} M_{jk} \theta_{j+2} \theta_{k+2}\right). \end{aligned}$$

Note that the first equality relied on  $\rho$  being even. Recalling the fermionic swap unitary (equation E.1) specialized to  $S = S_{1 \leftrightarrow 2n+1}$ , conjugation swaps the subspaces  $(1, 2) \leftrightarrow (2n+1, 2n+2)$  in the extended covariance matrix representation, then

$$(S_{1 \leftrightarrow 2n+1} \tau S_{1 \leftrightarrow 2n+1}^\dagger)(\theta) = \exp \left( \theta_{2n+1} + \sum_{j < k=1}^{2n} M_{jk} \theta_j \theta_k \right).$$

We further have  $\sigma = S_{1 \leftrightarrow 2n+1} \tau S_{1 \leftrightarrow 2n+1}^\dagger$  since fermionic swap  $S_{1 \leftrightarrow 2n+1}$  acts as a genuine swap gate if any of the two lines has definite parity (i.e. is part of an even state) and  $\rho$  is even. Matching the Fourier expression with the extended covariance matrix concludes the proof.  $\square$

**Theorem F.2** (restatement of theorem V.1). *Given a  $n$ -qubit state  $\rho$ ,  $\mathcal{E}(\rho) \in \mathbf{Gauss}(n+1) \iff \rho \in \mathbf{DGauss}(n)$ , in which case the covariance matrix of the embedding is*

$$\Sigma[\mathcal{E}(\rho)] = \begin{bmatrix} \Sigma(\rho) & -ir & i\mu(\rho) \\ ir^T & 0 & ic \\ -i\mu(\rho)^T & -ic & 0 \end{bmatrix} \in \mathfrak{so}(2n+2), \quad R = \begin{bmatrix} R_0 & s \\ r^T & c \end{bmatrix} \in SO(2n+1). \quad (\text{F.5})$$

Here  $r \in \mathbb{R}^{2n}$  and  $c \in \mathbb{R}$  are the entries of  $R$  such that  $R\tilde{\Sigma}(\rho)R^T$  is block-diagonal and trivial on the last subspace. Moreover,  $\rho$  is displaced Gaussian iff  $\mathcal{E}(\rho)$  is Gaussian.

*Proof.* Let  $\Sigma = \Sigma(\rho)$ ,  $\mu = \mu(\rho)$ . We first prove that that  $\rho \otimes |+\rangle\langle+|$  is a displaced Gaussian state: by theorem D.4, write  $\rho = U_G^\dagger \rho_D U_G$  for  $U_G \in DG(n)$  then  $U_G$  affects  $R$  that block-diagonalizes  $\tilde{\Sigma}(\rho)$ . Then  $\rho = U_G^\dagger \rho_D U$  implies

$$\rho \otimes |+\rangle\langle+| = (U_G^\dagger \otimes I)(\rho_D \otimes |+\rangle\langle+|)(U_G \otimes I)$$

is Gaussian since  $\rho_D \otimes |+\rangle\langle+|$  is Gaussian by lemma F.1. Decompose  $R$  in terms of  $R_0, r, c$  as in equation F.5, the rotation  $\bar{R} \in SO(2n+3)$  corresponding to  $U_G \otimes I$ , as well as the extended covariance matrix  $\tilde{\Sigma}(\rho \otimes I)$ , are

$$\bar{R} = \begin{bmatrix} R_0 & 0_{2n \times 2} & s \\ 0_{2 \times 2n} & I_{2 \times 2} & 0_{1 \times 2} \\ r^T & 0_{2 \times 1} & c \end{bmatrix}, \quad \tilde{\Sigma}(\rho \otimes I/2) = \begin{bmatrix} \Sigma & 0_{2n \times 2} & i\mu \\ 0_{2 \times 2n} & 0_{2 \times 2} & 0 \\ -i\mu^T & 0 & 0 \end{bmatrix} = \bar{R}^T \tilde{\Sigma}(\rho_D \otimes I/2) \bar{R}.$$

Recalling  $\tilde{\Sigma}(\rho_D \otimes |+\rangle\langle+|) = \tilde{\Sigma}(\rho_D \otimes I) + is_{(2n+1)(2n+3)}$  from lemma F.1, we obtain

$$\begin{aligned} \tilde{\Sigma}(\rho \otimes |+\rangle\langle+|) &= \bar{R}^T \left[ \tilde{\Sigma}(\rho_D \otimes |+\rangle\langle+|) \right] \bar{R} = \tilde{\Sigma}(\rho \otimes I/2) + i\bar{R}^T (|2n+1\rangle\langle 2n+3| - |2n+3\rangle\langle 2n+1|) \bar{R} \\ &= \tilde{\Sigma}(\rho \otimes I/2) + i \left( |2n+1\rangle \begin{bmatrix} r \\ 0_{1 \times 2} \\ c \end{bmatrix} - \begin{bmatrix} r^T & 0_{2 \times 1} & c \end{bmatrix} \langle 2n+1| \right) \\ &= \begin{bmatrix} \Sigma & -ir & 0_{2n \times 1} & i\mu \\ ir^T & 0 & 0 & ic \\ 0_{1 \times 2n} & 0 & 0 & 0 \\ -i\mu^T & -ic & 0 & 0 \end{bmatrix} \implies \tilde{\Sigma}[V(\rho \otimes |+\rangle\langle+|)V^\dagger] = \begin{bmatrix} \Sigma & -ir & i\mu & 0_{2n \times 1} \\ ir^T & 0 & ic & 0 \\ -i\mu^T & -ic & 0 & 0 \\ 0_{1 \times 2n} & 0 & 0 & 0 \end{bmatrix} \end{aligned}$$

The last implication holds because conjugation by  $V$  swaps the  $(2n+2)$  and  $(2n+3)$ -th subspaces in  $\tilde{\Sigma}(\rho \otimes |+\rangle\langle+|)$  using equation F.3. We obtain the desired covariance matrix relation by noting that  $\Sigma$  is the restriction to all but the last subspace. This establishes the forward direction in the equivalence; for the converse, suppose for contraposition that  $\mathcal{E}(\rho) = V(\rho \otimes |+\rangle\langle+|)V^\dagger$  is non-Gaussian; since  $V \in DG(n+1)$ , this implies that  $\rho \otimes |+\rangle\langle+|$  is non-Gaussian. But  $\rho_G \otimes |+\rangle\langle+|$  is displaced Gaussian if  $\rho_G$  is Gaussian by the reasoning above, so  $\rho$  cannot be displaced Gaussian.  $\square$

The even Gaussian state embedding has a corresponding compatible embedding for Gaussian unitaries.

**Lemma F.3** (restatement of lemma V.2). *Let  $U \in \mathcal{C}_{2n}$ , define  $\tilde{U} = V(U \otimes I)V^\dagger \in \mathcal{C}_{2n+2}$ , with  $V$  being the same unitary in the even embedding channel F.1, then for any  $\tilde{U}$  in the image of the transformation,*

$$U \in DG(n) \iff \tilde{U} \in G(n+1). \quad (\text{F.6})$$

The mean  $i\gamma^T d$  is transformed into covariance  $-i(\gamma^T d)\gamma_{2n+2}$ , and the Gaussian expressions are

$$U = \exp \left( \frac{1}{2} \gamma^T h \gamma + i\gamma^T d \right) \iff \tilde{U} = \exp \left( \frac{1}{2} \gamma^T \tilde{h} \gamma \right), \quad \tilde{h} = \begin{bmatrix} h & 0_{2n \times 1} & -d \\ 0_{1 \times 2n} & 0 & 0 \\ d^T & 0 & 0 \end{bmatrix}. \quad (\text{F.7})$$

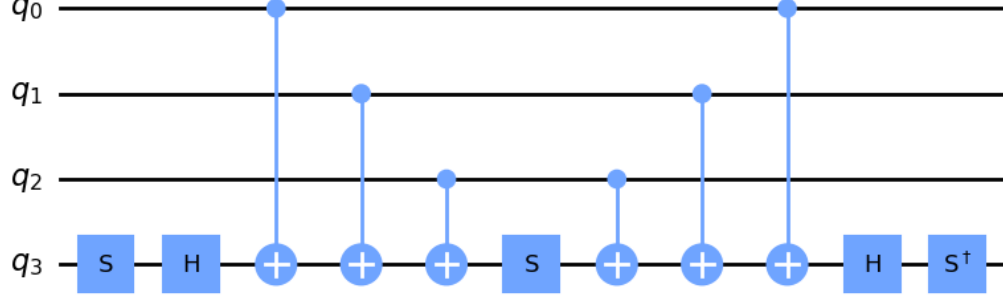


FIG. 1. Elementary decomposition of the even embedding unitary  $V$  (equation V.2) used to embed  $\mathbf{DGauss}(3)$ .

*Proof.* Note  $\phi(\gamma_j) = V\gamma_jV^\dagger$ . Since conjugation by  $V$  is unitary, it is extended multiplicatively just as  $\phi$ . Let  $\gamma = (\gamma_1, \dots, \gamma_{2n})$  and  $\tilde{\gamma} = (\gamma_1, \dots, \gamma_{2n+2})$ , then

$$\tilde{U} = \phi(e^{\log U}) = \exp \left[ \phi \left( \frac{1}{2} \gamma^T h \gamma + i \gamma^T d \right) \right] = \exp \left[ \frac{1}{2} \gamma^T h \gamma - (\gamma^T d) \gamma_{2n+1} \right] = \exp \left( \frac{1}{2} \tilde{\gamma}^T \tilde{h} \tilde{\gamma} \right).$$

□

We now proceed to decompose  $V \in DG(n+1)$  into products of elementary gates. Recalling  $S = \text{diag}(1, i)$ , let  $A = S^\dagger H$  and  $CX_{a \rightarrow b}$  denote the controlled-not with  $a$  as control and  $b$  as target. This yields the conjugation relations

$$AYA^\dagger = -Z, \quad (CX_{a \rightarrow b}) Z_b (CX_{a \rightarrow b}) = Z_a Z_b. \quad (\text{F.8})$$

Fixing  $n$ , let  $B = \prod_{j=1}^n CX_{j \rightarrow n+1}$  and letting  $\cong$  denote equivalence up to a global phase, we obtain:

$$\begin{aligned} ABS_{n+1}BA^\dagger &\cong AB \exp \left( i \frac{\pi}{4} Z_{n+1} \right) BA^\dagger = A \exp \left( i \frac{\pi}{4} Z_1 \dots Z_{n+1} \right) A^\dagger \\ &= \exp \left( -i \frac{\pi}{4} Z_1 \dots Z_n Y_{n+1} \right) = \exp \left( -i \frac{\pi}{4} \gamma_{2n+2} \right) = V \in DG(n). \end{aligned}$$

The  $n = 3$  case is illustrated in Fig. 1 using the Qiskit library [30].