Gaussian quantum operator representation for fermions

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We present a quantum operator representation for fermions, using the most general multi-mode Gaussian operator basis. The representation extends existing bosonic phase-space methods to Fermi systems. We derive results on completeness and positivity, as well as the existence of second-order differential identities for operator products. Grassmann integration is employed to prove the identities. However, the resulting phase space involves only c-numbers, without requiring anticommuting Grassmann variables. The representation thus enables first-principles dynamical or equilibrium calculations in quantum many-body Fermi systems.

I. INTRODUCTION

In this paper we address the issue of how to represent highly-correlated fermionic states. To this end, we introduce a general Gaussian operator basis for fermionic density operators. Like the analogous basis for bosons, the Gaussian basis enables a generalised phase-space representation of arbitrary physical density operators as a distribution over the phase-space. We prove three central results: the basis is complete, the distribution can always be chosen positive, and there are mappings to a second-order differential form for all operator products up to quartic order. Hence, positive-definite Fokker-Planck equations exist for many-body fermionic systems. This leads to first-principles stochastic simulation methods, either in real time or at finite temperature.

Phase-space representation is relevant to a longstanding problem in theoretical physics, which is the sign problem that occurs in many-body fermionic wave-functions. In general, fermionic sign problems manifest themselves in several ways. There are many different approximate techniques that can be used, but the intention of this paper is to establish fundamentally exact procedures to treat the Fermi sign problem. We shall proceed in two stages. The present paper derives the requisite formal identities required for the Gaussian representation method. A subsequent paper will establish techniques for using these identities in practical simulations of the Hubbard model and other related problems in fermionic many-body theory.

For bosonic systems, phase-space methods based on the positive-P distribution have proved a successful way to simulate quantum many-body systems from first-principles. These methods sample the time evolution of a positive distribution on an overcomplete basis set, which is usually the set of coherent states. They extend earlier approaches such as the Wigner function, the Q-function, the Glauber-Sudarshan P-function, and their generalizations. Coherent states for fermions were defined in a seminal paper by Cahill and Glauber using anticommuting Grassmann variables. These provide a means of defining quasi-probabilities for Fermionic states analogous to the well-known bosonic distributions. However, the resulting quasi-probabilities are functions of non-commuting Grassmann variables, and are not computationally accessible.

We introduce a phase-space representation that overcomes the problem of Grassmann complexity by using a Gaussian expansion for the density operator. This uses an operator basis constructed from pairs of Fermi operators, rather than a state-vector basis as in more usual approaches. This substantially generalizes and extends earlier related techniques used to treat electronic transitions in atoms. Because pairs of Fermi operators obey commutation relations rather than anti-commutation relations, a natural solution of the Grassmann problem is achieved. Furthermore, the resulting phase-space equations obviate the need to evaluate large determinants in simulations. The practical advantages of this representation were demonstrated in , in which we applied the method to the well-known Hubbard model and were able to overcome the sign problem.

We begin in Sec. by establishing the definition of a Gaussian operator, and giving elementary examples of one and two-mode Gaussians in order to explain our approach. Section introduces the set of most general normalized Gaussian operators and discusses some of its properties that are relevant to its use as a basis set. In Sec. we define the Gaussian representation as an expansion in Gaussian operators, and then show how the representation establishes a novel class of exact Monte-Carlo type methods for simulating the real-time dynamics or finite-temperature equilibrium of a quantum system. These properties are proved in Appendix by use of Fermi coherent states, which in turn are discussed in Appendix.

II. ELEMENTARY GAUSSIAN OPERATORS

To define Gaussian operators for a given fermionic system, we first decompose it into a set of orthogonal single-particle modes, or orbitals. With each of these modes, we associate creation and annihilation operators...
The simplest, unnormalized Gaussian which generalizes the usual thermal density matrix is therefore:

\[
\tilde{\Lambda}^{(u)}_M(\mu) = \exp\left[-\hat{b}^\dagger \mu \hat{b}\right] = \prod_{i,j=1}^{M} \exp\left[-\hat{b}^\dagger_i \mu_{ij} \hat{b}_j\right] = \prod_{i,j=1}^{M} \left[1 - \hat{b}^\dagger_i \mu_{ij} \hat{b}_j\right],
\]

(2.1)

where \( \mu \) is a complex \( M \times M \) matrix. The last result follows because normally ordered products in which the same operator appears more than once are zero, from the anti-commutation relations in Eq (2.2).

The most general form is a squeezed Gaussian:

\[
\tilde{\Lambda}^{(u)}_M(\mu, \xi, \xi^+) = \exp\left[-\hat{b}^\dagger \mu \hat{b} - \frac{1}{2} \left(\hat{b} \xi^+ \hat{b} + \hat{b}^\dagger \xi \hat{b}^\dagger\right)\right] = \prod_{i>j} \left[1 - \xi_{ij} \hat{b}^\dagger_i \hat{b}_j\right] \prod_{i<j} \left[1 - \mu_{ij} \hat{b}^\dagger_i \hat{b}_j\right] \times \prod_{i>j} \exp\left[1 - \xi^+_{ij} \hat{b}^\dagger_i \hat{b}_j\right].
\]

(2.2)

Here \( \xi, \xi^+ \) are complex antisymmetric \( M \times M \) matrices. Normalized forms \( \tilde{\Lambda}_M \), for which \( Tr(\tilde{\Lambda}_M) = 1 \), will be introduced later.

In order to relate these quadratic expressions to the usual Dirac state notation, we define number states as:

\[
|\vec{n}\rangle = |n_1\rangle \otimes |n_2\rangle \otimes \cdots \otimes |n_M\rangle = (\hat{b}^\dagger_1)^{n_1} (\hat{b}^\dagger_2)^{n_2} \cdots (\hat{b}^\dagger_M)^{n_M} |0\rangle_M,
\]

(2.4)

where \( \vec{n} = (n_1, n_2, \ldots, n_M) \) is a vector of integer occupations and where \( |0\rangle_M \) is the \( M \)-mode fermion vacuum state.

We also recall some elementary identities which relate quadratic forms in fermion operators to state projection operators. For individual operators, one has the well-known identities:

\[
\hat{b}_j = |0\rangle_j \langle 1|_j,
\]

\[
\hat{b}^\dagger_j = |1\rangle_j \langle 0|_j.
\]

(2.5)

Hence, the elementary identities for quadratic products are as follows, for \( i < j \):

\[
\hat{b}^\dagger_i \hat{b}_j = |1\rangle_i \langle 1|_i \prod_{k \neq i,j} \hat{b}_k,
\]

\[
\hat{b}_i \hat{b}^\dagger_j = |0\rangle_i \langle 0|_i \prod_{k \neq i,j} \hat{b}_k.
\]

(2.6)

where \( \hat{1}_k \) is the identity operator for the \( k \)-th mode.

In the rest of this section, we will establish some elementary results for the examples of one and two mode Gaussian operators.

**A. Single-mode Gaussian operators**

An unnormalized Gaussian operator for a single mode has only one possible form:

\[
\tilde{\Lambda}^{(u)}_1(\mu) = \exp\left[-\mu \hat{b}^\dagger \hat{b}\right] = \sum_{k=0}^{\infty} \frac{1}{k!} (-\mu \hat{b}^\dagger \hat{b})^k,
\]

(2.7)

where the exponential is defined, as indicated, by its series representation. Just as in the general case of Eq (2.2), the anticommutivity of the fermionic operators means that only the zeroth and first-order terms in the expansion contribute to the single mode Gaussian, giving the simple result:

\[
\tilde{\Lambda}^{(u)}_1(\mu) = 1 - \mu \hat{b}^\dagger \hat{b}.
\]

(2.8)

The normalisation of this Gaussian operator is

\[
N_1 = Tr \tilde{\Lambda}_1 = 2 - \mu.
\]

(2.9)

Excluding the point \( \mu = 2 \), we define the new parameter \( \eta = (1 - \mu)/(2 - \mu) \), which allows us to write the Gaussian
in normalised form as
\[ \hat{\Lambda}_1(n) = (1 - n) : \exp \left[ - (2 + 1/(n - 1)) \hat{b}^\dagger \hat{b} \right] : \]
\[ = (1 - n) \hat{b}^\dagger \hat{b} + n \hat{b}^\dagger \hat{b} \]
\[ = (1 - n) |0\rangle\langle 0| + n |1\rangle\langle 1|. \tag{2.10} \]

If \( n \) is real, then Eq. (2.10) shows directly that \( \hat{\Lambda}_1(n) \) is the density operator corresponding to a mixture of number states in the one-mode case. The expectation value of the fermion occupation \( \hat{n} \equiv \hat{b}^\dagger \hat{b} \) is just the variable \( n \).

1. Completeness and positivity

As two special cases we obtain the number states:
\[ |0\rangle\langle 0| = \hat{\Lambda}_1(0) \]
\[ |1\rangle\langle 1| = \hat{\Lambda}_1(1), \tag{2.11} \]
which implies that the single-mode Gaussians form a complete basis set for a number-conserving subset of Hilbert space. Because super-selection rules prohibit superpositions of states differing by odd numbers of fermions, this is the most general case possible. Furthermore, we see from Eq. (2.11) that the most general single-mode density matrix can be expanded as a mixture of Gaussians with positive coefficients:
\[ \hat{\rho} = \hat{\Lambda}_1(n) = (1 - n) \hat{\Lambda}_1(0) + n \hat{\Lambda}_1(1), \tag{2.12} \]
which proves the positivity of the Gaussians as a basis for a one-mode system.

The more general Gaussian operator, with \( n \) complex, provides an overcomplete basis for physical density matrices, even though such Gaussians are not in themselves physical density matrices. This means that a physical density matrix may be represented by more than one distribution over the Gaussians. For example, any uniform phase distribution over Gaussian states gives the vacuum:
\[ |0\rangle\langle 0| = \int d\phi \hat{\Lambda}_1(re^{i\phi}). \tag{2.13} \]

B. Two-mode number-conserving Gaussian operators

A straightforward extension of the generalized thermal Gaussian form to two modes gives
\[ \hat{\Lambda}_2^{(n)}(\mu) = : \exp \left[ - \sum_{i,j=1}^{2} \mu_{ij} \hat{b}_i^\dagger \hat{b}_j \right] : \]
\[ = 1 - \sum_{i,j=1}^{2} \mu_{ij} \hat{b}_i^\dagger \hat{b}_j + \det \mu \hat{b}_1^\dagger \hat{b}_2 \hat{b}_2^\dagger \hat{b}_1, \tag{2.14} \]
where the \( \mu_{ij} \) are the elements of the \( 2 \times 2 \) matrix \( \mu \). The last step follows by explicitly expanding the general result in Eq. (2.12), while taking account of the sign changes during normal ordering. Again, the series expansion contains all possible normally ordered nonzero products of the \( \hat{b}_1^\dagger \hat{b}_j \) pairs. In terms of two-mode number-state projectors, the Gaussian operator is
\[ \hat{\Lambda}_2^{(n)}(\mu) = |00\rangle\langle 00| + (1 - \mu_{11}) |10\rangle\langle 10| + (1 - \mu_{22}) |01\rangle\langle 01| + (1 - \mu_{11} - \mu_{22} + \det \mu) |11\rangle\langle 11| - \mu_{12} |10\rangle\langle 01| - \mu_{21} |01\rangle\langle 10|. \tag{2.15} \]

1. Normalisation and Moments

Following from Eq. (2.15), the normalisation is
\[ N_2 = 4 - 2\mu_{11} - 2\mu_{22} + \det \mu. \tag{2.16} \]
Defining the matrix \( \mathbf{n} = \mathbf{I} - (2\mathbf{I} - \mu^T)^{-1} \), where \( \mathbf{I} \) is the \( 2 \times 2 \) identity matrix, we can write the normalised two-mode Gaussian as
\[ \hat{\Lambda}_2(n) = \det [\mathbf{I} - \mathbf{n}] : \exp \left[ -\hat{\mathbf{b}}^\dagger (2\mathbf{I} + [\mathbf{n}^T - \mathbf{I}]^{-1}) \hat{\mathbf{b}} \right] : \]
\[ = \det [\mathbf{I} - \mathbf{n}] |00\rangle\langle 00| + (n_{11} - 1 - n_{22}) |10\rangle\langle 10| + (1 - n_{11} + n_{12}n_{21}) |01\rangle\langle 01| + \det \mathbf{n} |11\rangle\langle 11| + n_{21} |10\rangle\langle 01| + n_{12} |01\rangle\langle 10|. \tag{2.17} \]

If \( n \) is an Hermitian matrix, then the two-mode Gaussian corresponds to the density matrix of a mixture of states of different total number, with coherences \( n_{12} = n_{21} \) between states of the same total number.

Normally ordered first-order correlations of the Gaussian density matrices correspond to elements of \( \mathbf{n} \):
\[ \left\langle \hat{b}_i^\dagger \hat{b}_j \right\rangle_\Lambda = \text{Tr} \hat{b}_i^\dagger \hat{b}_j \hat{\Lambda}_2 = n_{ij}, \tag{2.18} \]
and higher-order correlations reduce to products of first-order averages, for example,
\[ \left\langle \hat{b}_1^\dagger \hat{b}_1 \hat{b}_2 \hat{b}_2 \right\rangle_\Lambda = n_{11}n_{22} - n_{12}n_{21}. \tag{2.19} \]

This kind of factorisation of higher-order correlations could be taken as the defining characteristic of a Gaussian state, and more generally, Gaussian operators, rather than the more formal operator definition given by Eq. (2.14). In other words, Gaussian operators have both a Gaussian form and generate Gaussian statistics. The connection between these two defining features can be made more explicit by use of a moment-generating function, or characteristic function, which is considered in Appendix C.
Because the matrix $\mathbf{n}$ is Hermitian for a Gaussian that is a density operator, it can be diagonalised, corresponding to a change of single-particle basis. In this diagonalised basis, since the coherences are zero, the density operator is a mixture of number states, totally characterised by average occupation numbers. In other words, these Gaussian operators, given by Eq. (2.21), correspond to two-mode thermal states.

2. Completeness and positivity

We wish to show that any number-conserving two-mode density matrix can be expanded in terms of Gaussian operators, with positive expansion coefficients. This follows if we can represent all the number-state projectors between states of the same total number using Gaussian operators. By inspection of Eq. (2.17), above, we find that:

$$
\rho_{n_0} = \tilde{\Lambda}_2(0),
$$

$$
\rho_{10} = \tilde{\Lambda}_2(10),
$$

$$
\rho_{01} = \tilde{\Lambda}_2(0 1),
$$

$$
\rho_{11} = \tilde{\Lambda}_2(1 1),
$$

$$
\rho_{n_0 \rho_{10}} = \tilde{\Lambda}_2(n_{21} 10),
$$

$$
\rho_{n_0 \rho_{01}} = \tilde{\Lambda}_2(n_{12} 0 1),
$$

$$
\rho_{n_0 \rho_{11}} = \tilde{\Lambda}_2(n_{21} 0 n_2),
$$

$$
\rho_{10 \rho_{01}} = \tilde{\Lambda}_2(n_{12} n_{21}),
$$

$$
\rho_{10 \rho_{11}} = \tilde{\Lambda}_2(n_{12} n_{21}),
$$

$$
\rho_{10 \rho_{10}} = \tilde{\Lambda}_2(n_{12} n_{21}).
$$

(2.20)

Thus, the two-mode Gaussians form a complete operator basis for all number-conserving density matrices. For example, any uncorrelated product of number states mixtures can be represented exactly:

$$
\tilde{\rho}_{n_0} \otimes \tilde{\rho}_{n_2} = \tilde{\Lambda}_2(n_{21} 10, n_{12} 0 1).
$$

(2.21)

As well as these uncorrelated mixtures, the Gaussian basis can also be used to represent a mixture with correlations between the modes, this time as a sum (with positive weights) of two terms:

$$
A|00\rangle \langle 00| + B|11\rangle \langle 11| = A\tilde{\Lambda}_2(0) + B\tilde{\Lambda}_2(1).
$$

(2.22)

Superpositions of number states can also be represented, subject to total-number conservation. Thus the density matrix corresponding to the state $|\phi\rangle = \alpha |10\rangle + \beta |01\rangle$ is

$$
|\phi\rangle \langle \phi| = |\alpha|^2 |10\rangle \langle 01| + |\beta|^2 |01\rangle \langle 01| + \alpha^* \beta |10\rangle \langle 10| + \alpha \beta^* |01\rangle \langle 01| = \tilde{\Lambda}_2\left(\frac{|\alpha|^2}{|\beta|^2}, \frac{\alpha^* \beta}{|\beta|^2}, |\beta|^2\right).
$$

(2.23)

Not only is the two-mode Gaussian a complete representation, but it is also a positive one: any two-mode number-conserving density operator can be written as a positive distribution over Gaussian operators. To see this, note that while the expression for the projection operators, Eq. (2.24), includes terms with negative coefficients, the projectors involved are the off-diagonal ones. Since density matrices are positive-definite, off-diagonal projectors can only occur in combination with diagonal projectors.

Taking this into account, we find that any two-mode density operator can be expanded into number-state projector operators as follows:

$$
\tilde{\rho} = \sum_{n, n'} \rho_{n, n'} |\tilde{n}\rangle \langle \tilde{n'}|.
$$

(2.24)

where $\tilde{n}$ and $\tilde{n'}$ are vectors of integer occupation numbers: $\tilde{n} = (n_1, n_2)$, $\tilde{n'} = (n'_1, n'_2)$. Here $\rho_{n, n'} = 0$ if $\sum_j n_j \neq \sum_j n'_j$. Using the relations in Eq. (2.20), we can write the density operator as

$$
\tilde{\rho} = \sum_{n} \frac{1}{Z} \rho_{n, n} \tilde{\Lambda}_2\left(n_1, n_2\right).
$$

(2.25)

Since the diagonal coefficients $\rho_{n, n}$ are positive and sum to one, the Gaussian operators form the basis of a probabilistic representation of any two-mode density operator.

C. Two-mode squeezed Gaussian operators

Equation (2.17) does not represent the most general two-mode Gaussian form, as the quadratic form does not yet include terms such as $b_{1\dagger} b_{2\dagger}$. Incorporating such anomalous products, we can write the most general Gaussian operator in normalised form as:

$$
\tilde{\Lambda}_2^{(w)}(\mu, \xi, \xi^+) = \exp \left[ - \sum_{i,j=1}^2 \mu_{ij} b_{i\dagger} b_j - \xi^+ b_{1\dagger} b_2 - \xi b_{2\dagger} b_1 \right] = 1 - \sum_{i,j=1}^2 \mu_{ij} b_{i\dagger} b_j - \xi^+ b_{1\dagger} b_2 - \xi b_{2\dagger} b_1,
$$

(2.26)

where $\xi$ and $\xi^+$ are independent complex numbers. The two additional operator terms in the expansion, $b_{1\dagger} b_{2\dagger}$ and $b_{2\dagger} b_{1\dagger}$, are projectors between states of different total number:

$$
\tilde{b}_{1\dagger} b_2 = - |00\rangle \langle 11|,
$$

$$
\tilde{b}_{2\dagger} b_1 = - |11\rangle \langle 00|.
$$

(2.27)

which are the kinds of coherences that appear in the density matrices of two-mode squeezed states.
1. Normalisation and Moments

The normalisation of the squeezed Gaussian is

$$N_s = 4 - 2\mu_{11} - 2\mu_{22} + \det \mu + \xi^+.$$ \hfill (2.28)

To incorporate this into a normalised Gaussian, we redefine the $\mathbf{n}$ matrix to be

$$\mathbf{n} = \mathbf{I} - \frac{N_s}{N_s - \xi^+} (2\mathbf{I} - \mu^T)^{-1},$$ \hfill (2.29)

and introduce rescaled squeezing parameters $m = -\xi/N_s$, $m^+ = -\xi^+/N_s$. The normalised form is then

$$\hat{\Lambda}_2(\mathbf{n}, m, m^+) = (\det [\mathbf{I} - \mathbf{n}] + mm^+) \times \exp \left( \hat{b}^\dagger \hat{b} \right) (\mathbf{I} - \mathbf{a}^{-1}/2) \left( \hat{b} \hat{b}^T \right),$$ \hfill (2.30)

where the $4 \times 4$ matrices $\mathbf{I}$ and $\mathbf{a}$ are defined to be

$$\mathbf{I} = \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix},$$

$$\mathbf{a} = \begin{bmatrix} n_{11} - 1 & n_{21} & 0 & m \\ n_{12} & n_{22} - 1 & -m & 0 \\ 0 & -m^+ & 1 - n_{11} & -n_{12} \\ m^+ & 0 & -n_{21} & 1 - n_{22} \end{bmatrix}. \hfill (2.31)$$

In terms of number-state projectors, the normalised Gaussian is a generalisation of the number-conserving case, but with the additional non-number-conserving projectors:

$$\hat{\Lambda}_2(\mathbf{n}) = (\det [\mathbf{I} - \mathbf{n}] + mm^+) \langle 00 | 00 \rangle + (n_{11}(1 - n_{22}) + n_{12}n_{21} - mm^+) \langle 10 | 10 \rangle + (n_{22}(1 - n_{11}) + n_{12}n_{21} - mm^+) \langle 01 | 01 \rangle + (\det \mathbf{n} + mm^+) \langle 11 | 11 \rangle + n_{21} \langle 10 | 01 \rangle + n_{12} \langle 01 | 10 \rangle - m \langle 11 | 00 \rangle - m^+ \langle 00 | 11 \rangle.$$ \hfill (2.32)

In addition to the normal fluctuations of Eq. (2.18), the squeezed Gaussians also contain anomalous fluctuations, which are just equal to the new variables $m$ and $m^+$:

$$\langle \hat{b}_1 \hat{b}_2 \rangle = m,$$

$$\langle \hat{b}_1^\dagger \hat{b}_2^\dagger \rangle = m^+,$$ \hfill (2.33)

which implies that, for $\hat{\Lambda}_2(\mathbf{n}, m, m^+)$ to be a density matrix, $m$ and $m^+$ must be complex-conjugate. The second-order correlation generalises to

$$\langle \hat{b} \hat{b}_1 \hat{b}_2 \hat{b}_2 \rangle = n_{11}n_{22} - n_{12}n_{21} + mm^+, \hfill (2.34)$$

which again corresponds to the decorrelation that occurs in a state with Gaussian statistics.

2. Completeness and Positivity

From Eq. (2.30), it follows that the squeezed Gaussians provide a complete basis, not only for the number-conserving subspace, but also for all states containing superpositions of states whose difference in total number is even. To see this, note that the projectors between number the $|00\rangle$ and $|11\rangle$ number states can be written explicitly in terms of the Gaussian operators as

$$m |11\rangle \langle 00 | = \hat{\Lambda}_2(\mathbf{n}, -m, 0) - \hat{\Lambda}_2(\mathbf{n}, 0, 0),$$

$$m^+ |00\rangle \langle 11 | = \hat{\Lambda}_2(\mathbf{n}, 0, -m^+) - \hat{\Lambda}_2(\mathbf{n}, 0, 0),$$ \hfill (2.35)

for any $\mathbf{n}$. These projectors, together with those of Eq. (2.20), span the complete Hilbert space of density matrices in question.

As an example of the additional kinds of physical states that the squeezed Gaussians can represent, consider the non-number-conserving superpostion $|\Psi\rangle = (|00\rangle + |11\rangle) / \sqrt{2}$. Its corresponding density matrix is

$$\hat{\rho} = \frac{1}{2} (|00\rangle \langle 00 | + |11\rangle \langle 00 | + |00\rangle \langle 11 | + |11\rangle \langle 11 |) = \hat{\Lambda}_2\left(\mathbf{1}, -\frac{1}{2}, -\frac{1}{2}\right). \hfill (2.36)$$

As for the number-conserving case, we can write any physical density operator as a positive distribution over Gaussian operators:

$$\hat{\rho} = \sum_n \sum_{n'} \rho_{n,n'} |n\rangle \langle n'|$$

$$= \sum_n \frac{1}{2} \rho_{n,n} \times \hat{\Lambda}_2\left(\mathbf{1}, 2\rho_{(01),(10)} n_{12}, -2\rho_{(11,00)}, 0\right) + \hat{\Lambda}_2\left(\mathbf{1}, 2\rho_{(10),(01)} n_{12}, 0, -2\rho_{(00,11)}\right).$$

Thus the Gaussians form the basis of a probabilistic representation of any physical two-mode density operator. The ability to represent physical density matrices with the Gaussian basis, either as a single element or by a positive distribution over basis elements, is important for calculating dynamical simulations of quantum systems, as we discuss below in Sec. VII.

III. MULTIMODE DECOMPOSITION OF FERMI SYSTEMS

So far we have considered only one- and two-mode systems, to illustrate the basic physical properties of Gaussian operators. As we saw, the Gaussian operators could easily be written in terms of number-state projectors. The power of the Gaussian operators as a basis in its
own right becomes apparent for multimode systems, for which the number-state basis becomes unusable.

Before defining the general Gaussian basis for a system with many degrees of freedom, we define some mathematical notation and conventions that will be of subsequent use. As before, we define \( \hat{b} \) as a column vector of the \( M \) annihilation operators, and \( \hat{b}^\dagger \) as a row vector of the corresponding creation operators. We also introduce an extended column vector of all \( 2M \) operators: \( \hat{\mathbf{b}} = (\hat{b}^T, \hat{b}^\dagger)^T \), with an adjoint row vector defined as \( \hat{\mathbf{b}}^\dagger = (\hat{b}^\dagger, \hat{b}^T) \). Writing these out in full, we get:

\[
\hat{\mathbf{b}} = \begin{pmatrix}
\hat{b}_1 \\
\vdots \\
\hat{b}_M \\
\end{pmatrix}, \quad \hat{\mathbf{b}}^\dagger = \left( \hat{b}_1^\dagger, ..., \hat{b}_M^\dagger, \hat{b}_1, ..., \hat{b}_M \right). \tag{3.1}
\]

Throughout the paper, we print length-\( M \) vectors and \( M \times M \) matrices in bold type, and index them where necessary with Latin indices: \( j = 1, ..., M \). Length-\( 2M \) vectors we denote with an underline and \( 2M \times 2M \) matrices we denote with a double underline. These extended vectors and matrices are indexed where necessary with Greek indices: \( \mu = 1, ..., 2M \). Note that an object such as \( \hat{\mathbf{b}} \hat{\mathbf{b}}^\dagger \) is a \( 2M \times 2M \) matrix:

\[
\hat{\mathbf{b}} \hat{\mathbf{b}}^\dagger = \begin{bmatrix}
\hat{b} \hat{b}^\dagger & \hat{b} \hat{b}^T \\
\hat{b}^T \hat{b} & \hat{b}^T \hat{b}^T
\end{bmatrix}, \tag{3.2}
\]

whereas \( \hat{\mathbf{b}} \hat{\mathbf{b}} \) is a scalar. More general kinds of vectors are denoted with an arrow notation: \( \vec{\mu} \).

For products of operators, we make use of normal and antinormal ordering concepts. Normal ordering, denoted by \( \cdots \vdash \cdots \), is defined as in the bosonic case, with all annihilation operators to the right of the creation operators, except that each pairwise reordering involved induces a sign change, e. g., \( \hat{b}_i \hat{b}_j : = - \hat{b}_j \hat{b}_i \). The sign changes are necessary so that the anticommuting nature of the Fermi operators can be accommodated without ambiguity. We define antinormal ordering similarly, and denote it via curly braces: \( \{ \hat{b}_i \hat{b}_j \} = - \hat{b}_j \hat{b}_i \). More generally, we can define nested orderings, in which the outer ordering does not reorder the inner one. For example, \( \{ \hat{O} \hat{b}_i \hat{b}_j \} : = - \hat{b}_j \hat{b}_i \hat{O} : \), where \( \hat{O} \) is some operator.

For example, the different orderings of pairs are, in block matrix form,

\[
\begin{align*}
 : \hat{b}_\mu \hat{b}_\nu : & = : - \hat{b}_\nu \hat{b}_\mu : \\
\{ \hat{b}_\mu \hat{b}_\nu \} & = \{ - \hat{b}_\nu \hat{b}_\mu \} . \tag{3.3}
\end{align*}
\]

Note that this convention means that the relation between the two orderings is

\[
: \hat{b} \hat{b}^\dagger : = \mathbb{I} + \{ \hat{b} \hat{b}^\dagger \}, \tag{3.4}
\]

where \( \mathbb{I} \) is the constant matrix

\[
\mathbb{I} = \begin{bmatrix}
-\mathbf{I} & \mathbf{0} \\
\mathbf{0} & \mathbf{I}
\end{bmatrix}, \tag{3.5}
\]

in which \( \mathbf{0} \) and \( \mathbf{I} \) are the \( M \times M \) zero and identity matrices, respectively.

When ordering products that contain a Gaussian operator \( \Lambda \) (and later the density operator), we do not change the ordering of \( \Lambda \) itself; the other operators are merely reordered around it. Thus \( \{ \Lambda \hat{b}_i \hat{b}_j \} = - \hat{b}_j \hat{b}_i \Lambda \). The different possible quadratic orderings containing a Gaussian operator can thus be written in matrix form as

\[
\begin{align*}
: \hat{b} \hat{b}^\dagger \Lambda : & = \begin{bmatrix}
- (\hat{b} \Lambda \hat{b})^T & \hat{b} \Lambda \hat{b}^T \\
\hat{b} \Lambda \hat{b}^T & \hat{b} \Lambda \hat{b}^T
\end{bmatrix}, \\
\{ \hat{b} \hat{b}^\dagger \Lambda \} & = \begin{bmatrix}
\hat{b} \Lambda \hat{b}^T & \hat{b} \Lambda \hat{b}^T \\
\hat{b} \Lambda \hat{b}^T & - \hat{b} \Lambda \hat{b}^T
\end{bmatrix}, \\
\{ \Lambda \hat{b} \hat{b}^\dagger \} & = \begin{bmatrix}
\Lambda \hat{b} \hat{b}^T & - \hat{b} \Lambda \hat{b}^T \\
\hat{b} \Lambda \hat{b}^T & - \hat{b} \Lambda \hat{b}^T
\end{bmatrix} . \tag{3.6}
\end{align*}
\]

IV. GENERAL GAUSSIAN OPERATORS

A. Definition

We define a Gaussian operator \( \Lambda \) to be the most general Gaussian form of fermionic annihilation and creation operators, with zero displacement. Using the extended-vector notation, we can write the unnormalized Gaussian as

\[
\Lambda^{(u)}(\mu, \xi, \xi^+) : = \exp \left[ \frac{1}{2} \mathbf{b}^\dagger \left( \mathbf{I} - \mathbf{g}^{-1}/2 \right) \mathbf{b} \right] 
\]

where we have introduced a new extended \( 2M \times 2M \) covariance matrix \( \mathbf{g} \) defined in terms of \( \mu, \xi, \xi^+ \) so that:

\[
\mathbf{g}^{-1} = 2 \mathbb{I} + \left[ \begin{array}{cc}
\mu & \xi \\
\xi^T & -\mu^T
\end{array} \right] \tag{4.2}
\]

The introduction of the generalized covariance \( \mathbf{g} \) allows the matrix to be written in a normalised form, using the
results of Appendix B together with an explicit complex amplitude factor $\Omega$. With these definitions, the general Gaussian operator is:

$$\hat{\Lambda}(\lambda) = \Omega \text{Pf} \left[ \sigma_A \right] : \exp \left[ \frac{\hat{b}^\dagger \left( \mathbf{I} - \sigma^{-1} \right) \hat{b}}{2} \right] : .$$

(4.3)

Here, we have introduce a new parameterization of:

$$\lambda = (\Omega, n, m, m^+) ,$$

(4.4)

which allows us to work directly with the physically significant $M \times M$ submatrices of the covariance $\sigma$:

$$\sigma = \begin{bmatrix} n^T - \mathbf{I} & m & m^+ \\ m & \mathbf{I} - n \end{bmatrix} .$$

(4.5)

Here $n$ is a complex $M \times M$ matrix, which corresponds to the normal Green’s function in many-body terminology, while $m$ and $m^+$ are two independent antisymmetric complex $M \times M$ matrices that correspond to anomalous Green’s functions, as we will show in the next section. There are $1 + p = 1 + M(2M - 1)$ parameters in all.

One obvious difference with the conventional complex-number or bosonic Gaussian forms is the normalisation. Chosen to ensure that $\text{Tr} \hat{\Lambda} = \Omega$, it contains the Pfaffian of an antisymmetric form $\sigma_A$ of the covariance. The choice of anti-symmetrisation is given in Appendix B; other choices will lead, in general, to additional sign factors. Now the square of the Pfaffian of an antisymmetric matrix is equal to its determinant, and the determinant of $\sigma_A$ differs from that of $\sigma$ by a constant sign (see Appendix B). Thus $| \text{Pf} [\sigma_A] | = | \sqrt{\det \sigma} |$, and as we shall see, the relative phase between the two does not appear in later identities. The additional variable $\Omega$ plays the role of a weighting factor in the expansion that allows us to represent unnormalised density operators and to introduce ‘stochastic gauges’.

The covariance has a type of generalized Hermitian antisymmetry, which can be written as $\sigma = -\sigma^+$, with the definition that:

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix}^+ = \begin{bmatrix} d & c \\ b & a \end{bmatrix}^T .$$

(4.6)

It is this generalised antisymmetry that allows the covariance to be transformed into an explicitly antisymmetric matrix.

An important subset of the Gaussian operators is the set of generalised thermal states, for which $m = m^+ = 0$. In this case, from Appendix B and using the result that $[2\mathbf{I} - \lambda] = \left[ \mathbf{I} - n \right]^{-1}$, the normalization factor is $\det \left[ \mathbf{I} - n \right]$. The normalized thermal Gaussians therefore can be written:

$$\hat{\Lambda}(\lambda) = \Omega \det [\mathbf{I} - n] : \exp \left[ -\hat{b}^\dagger \left( 2\mathbf{I} + \left( n^T - \mathbf{I} \right)^{-1} \right) \hat{b} \right] : .$$

(4.7)

In order to use the Gaussian operator basis, we need to make use of a number of basic results. Their proofs can be established, as we show in Appendix B with Fermi coherent states and Grassmann algebra, the basics of which are given in Appendix A. However the final results do not contain any Grassmann variables.

### B. Trace Properties

Some basic traces are

$$\text{Tr} [\hat{\Lambda}] = \Omega ,$$

$$\text{Tr} [\hat{b}^\dagger \hat{b} \hat{\Lambda}] = 0 ,$$

$$\text{Tr} [\hat{b} \hat{b}^\dagger \hat{\Lambda}] = \Omega \sigma .$$

(4.8)

The first of these is the normalisation, proved as theorem 1 in Appendix B. That the second is zero follows from the fact that the Gaussians are constructed from pairs of ladder operators and thus cannot correspond to a superposition of states whose total fermion numbers differ by one. The same result holds for the trace with any odd product. The third trace, proved as theorem 2 in Appendix B, allows us to calculate first-order moments. In terms of the $M \times M$ submatrices, these become:

$$\text{Tr} [\hat{b}_i^\dagger \hat{b}_j \hat{\Lambda}] = \Omega n_{i,j} ,$$

$$\text{Tr} [\hat{b}_i \hat{b}_j \hat{\Lambda}] = \Omega m_{i,j} ,$$

$$\text{Tr} [\hat{b}_i \hat{b}_j^\dagger \hat{\Lambda}] = \Omega m_{i,j}^+ .$$

(4.9)

These results imply that for $\hat{\Lambda}$ itself to correspond to a physical density matrix, $n$ must be a Hermitian matrix, since $\langle \hat{b}_i^\dagger \hat{b}_j \rangle^* = \langle \hat{b}_j^\dagger \hat{b}_i \rangle$, and $m^+$ must be the Hermitian conjugate matrix of $m$, since $\langle \hat{b}_i \hat{b}_j \rangle^* = \langle \hat{b}_j \hat{b}_i \rangle$. Physically, $n$ gives the number, or normal, correlations, and $m$ and $m^+$ give the squeezing, or anomalous, correlations.

Another restriction on $\hat{\Lambda}$ being a physical density matrix that follows from Eq. (4.9) is that the eigenvalues of the matrix $n$ lie in the interval $[0, 1]$, because of the Pauli exclusion principle for fermions. Furthermore, the variance in the number correlations is

$$\text{var} \left\{ \langle \hat{b}_i^\dagger \hat{b}_j \rangle \right\} = \langle \hat{b}_i^\dagger \hat{b}_j \rangle \left( 1 - \langle \hat{b}_i^\dagger \hat{b}_j \rangle \right) ,$$

(4.10)

which implies that if all the eigenvalues of $n$ are 0 or 1, then $\hat{\Lambda}$ is a number state, as the variance in number
vanishes. If the eigenvalues are not limited to 0 or 1, then the \( \Lambda \) corresponds to a mixture of number states in the eigenbasis and is thus a (possibly squeezed) thermal state, characterised by average occupation numbers \( \overline{n}_j = \text{eig}_j(\Omega) \), and squeezing matrix \( m \).

A general Gaussian operator will not necessarily fulfill the Hermiticity condition and thus will not necessarily correspond to a physical state. However the set of operators that do correspond to physical states is an important subclass, because the expansion allows these states to be represented with exact precision. The inclusion of nonphysical states in the expansion, on the other hand, makes the Gaussian basis an (over)complete basis in which to expand a physical density operator of an arbitrary state (This is proved in Appendix B for the general case). The overcompleteness of the Gaussian operators as a basis set has important implications for representing arbitrary states with a positive distribution function, as we show below.

### C. Completeness and Positivity

We next wish to show that the previous results on completeness and positivity obtained for one and two mode density matrix representations can be generalized to the multi-mode case. That is, we will prove that:

- For any physical density matrix \( \hat{\rho} \), a positive set of coefficients \( P_j \) exists s.t.

\[
\hat{\rho} = \sum_j P_j \Lambda(\underline{\omega}^{(j)}) .
\]  

(4.11)

This central result does not rely on utilising the complex amplitudes \( \Omega \), which are part of the most general Gaussian operator. If these were used, then positivity of the coefficients would be trivial, since these additional amplitudes could be used to absorb any phase or sign factors arising in the expansion. Instead, we wish to prove a much stronger result, that a positive expansion exists without any additional amplitude factors. This result is analogous to a similar result known for the positive-P bosonic representation.

From the number state basis of Eq (2.4), the full set of possible fermionic many-body number states is the set \( \{|\vec{n}\rangle\} \) where \( \vec{n} \) is varied over all \( 2^M \) possible permutations. This defines a complete operator basis of dimension \( 2^{2M} \) for the set of all fermionic operators. While not all fermionic operators are Hermitian, it is no restriction to use this larger set of operators as a basis for the density matrices \( \hat{\rho} \).

Next, expand:

\[
\hat{\rho} = \sum_{\vec{n}} \sum_{\vec{m}} |\vec{n}\rangle \langle \vec{m}| \hat{\rho} |\vec{m}\rangle \langle \vec{n}| \\
= \sum_{\vec{n}} \sum_{\vec{m}} \rho_{\vec{n}\vec{m}} |\vec{n}\rangle \langle \vec{m}| \\
= \sum_{\vec{n}} \sum_{\vec{m}} \hat{\rho}_{\vec{n}\vec{m}}
\]

(4.12)

The positive definiteness of the density operator means in particular that diagonal density matrix elements are real and positive: \( \rho_{\vec{n}\vec{m}} > 0 \). It is sufficient for completeness to prove that any elementary fermionic operator of form \( \hat{\rho}_{\vec{n}\vec{m}} = \rho_{\vec{n}\vec{m}} |\vec{n}\rangle \langle \vec{m}| \) corresponds to a normalised Gaussian \( \Lambda(\Lambda) \), apart from a scaling factor which is positive. The demonstration proceeds by constructing limiting cases of Gaussians that correspond to each of the elementary components of the density matrix. As demonstrated in the one and two mode cases, such expansions are not unique, and generally one can obtain other more compact representations by combining diagonal and off-diagonal elements.

To prove the elementary result, we proceed in three steps:

1. **Diagonal operators**

The generic diagonal operator in the number basis is:

\[
\hat{\rho}_{\vec{n}\vec{m}} = \rho_{\vec{n}\vec{m}} |\vec{n}\rangle \langle \vec{m}| \\
= \rho_{\vec{n}\vec{m}} \prod_i |n_i\rangle_i \langle n_i|_i ,
\]

with a total occupation number

\[
N = \sum_i n_i .
\]

(4.13)

Each diagonal multi-mode projector \( |\vec{n}\rangle \langle \vec{n}| \) is simply an outer-product of single-mode density matrices. From the single-mode example in Section II A each single-mode density matrix corresponds to a Gaussian as in Eq (2.12). Thus, we see that a diagonal projector is exactly equal to a normalized Gaussian (we suppress the trivial arguments for simplicity):

\[
|\vec{n}\rangle \langle \vec{n}| = \prod_i \hat{\Lambda}_i |n_i| \\
= \hat{\Lambda}_M [\underline{n}] ,
\]

(4.14)

(4.15)

where the matrix \( \underline{n} \) is defined as \( n_i = n_i \delta_{ij} \).

Since we know that \( \rho_{\vec{n}\vec{m}} \) is real and positive, this shows that a positive Gaussian expansion exists for all diagonal density matrices:

\[
\hat{\rho}_{\vec{n}\vec{m}} = \rho_{\vec{n}\vec{m}} \hat{\Lambda}_M [\underline{n}] .
\]

(4.16)

In summary, a diagonal multi-mode projector \( |\vec{n}\rangle \langle \vec{n}| \) is simply an outer-product of single-mode density matrices, and hence corresponds exactly to a multi-mode normalized Gaussian.
2. Generalized thermal operators

We define generalized off-diagonal thermal operators as components of the density matrix such that

$$
\sum_i n_i = N = \sum_i m_i .
$$

(4.17)

These have the generic form:

$$
\hat{\rho}_{\vec{n} \vec{m}} = \rho_{\vec{n} \vec{m}} |\vec{n} \rangle \langle \vec{m}|.
$$

(4.18)

Consider the quasi-thermal explicitly Gaussian operator, defined so that $\xi, \xi^* = 0$ — that is, without exponentiated terms involving pairs of annihilation or creation operators. Let

$$
n'_i = \delta_{ij} \min\{n_i, m_i\},
$$

(4.19)

and define an off-diagonal Gaussian in terms of the diagonal normalized Gaussian:

$$
\tilde{\Lambda}^{(o)}(\mu, \nu') = \prod_{i \neq j} \left[1 - \mu_{ij} \hat{b}_i \hat{b}_j\right] \tilde{\Lambda}[\nu'] .
$$

(4.20)

Next, for every distinct mode $i$ with $\delta n_i = n_i - n'_i = 1$ one can define a corresponding distinct index $j(i)$ with $\delta m_j = m_j - m'_j = 1$. It follows from the minimum condition, Eq (4.19) that $j(i) \neq i$, and from the number-conservation equation, Eq (4.22), we have

$$
\sum_i \delta n_i = \sum_i \delta m_i .
$$

(4.21)

Similarly, for every distinct pairs of indices $i, i'$ with $\delta n_i = \delta n_{i'} = 1$, it follows that $j(i') \neq i$, since otherwise $\delta n_i = 0$. The mapping therefore generates distinct pairs so that $j(i) \neq j(i') \iff i \neq i'$. Next, we note that this mapping is not a permutation of the set of modes $i$ with $\delta n_i = 0$, since if it were the condition that $j(i') \neq i$ would be violated for some $i'$. Similarly, the mapping is not a permutation of any subset of these modes. This means that the only non-vanishing terms in the normalization factor $\det[2I - \Lambda]$ are the diagonal terms, which are already normalized.

Define the resulting set of $\delta M \leq M$ pairs as $\sigma = \{i, j\}$ , and let:

$$
\mu_{ij}(\epsilon, \vec{n}) = \sum_{\{i', j'\} \in \sigma} \frac{\mu_{i'i'j'j}}{-\epsilon},
$$

where $\mu^{\delta M} = \rho_{\vec{n} \vec{m}}$, so that:

$$
\tilde{\Lambda}[\mu(\epsilon), \vec{n}'] = : \prod_{i \neq j} \left[1 - \mu_{ij} \hat{b}_i \hat{b}_j\right] \tilde{\Lambda}[\vec{n}'] :
$$

$$
=: \prod_{\{i, j\} \in \sigma} \left[1 + \frac{\mu_{ij} \hat{b}_i \hat{b}_j}{\epsilon}\right] |\vec{n}'\rangle \langle \vec{n}'| .
$$

(4.22)

Next, consider the limit of $\epsilon \to 0$, so that to leading order,

$$
\hat{\rho}_{\vec{n} \vec{m}'} = \mu^{\delta M} : \prod_{\{i, j\} \in \sigma} \left[\hat{b}_i \hat{b}_j\right] |\vec{n}'\rangle \langle \vec{n}'| :
$$

$$
= \lim_{\epsilon \to 0} \epsilon^{S + \delta M} \tilde{\Lambda}^{(s)}[\mu(\epsilon), \xi(\epsilon), \vec{n}'].
$$

(4.23)

Again, we see that a positive expansion parameter is obtained.

3. Squeezed operators

We define squeezed operators as components $\rho_{\vec{n} \vec{m}}$ of the density matrix such that

$$
N = \sum_i n_i = \sum_i m_i + 2S ,
$$

(4.24)

where $S$ is an integer denoting the number of fermion pairs that change. We suppose that $S > 0$, since the case of $S < 0$ is obtained trivially by hermitian conjugation. Let $\vec{n}_i$ be obtained from $n_i$ by removing $2S$ occupied sites, labeled as successive pairs $i, j$ belonging to a set $\bar{\sigma}$, so that $\vec{N} = \sum_{i} \vec{n}_i = \sum_{i} n_i$. The occupation numbers $\vec{n}_i, m_i$ now define a generalised thermal density matrix component as previously, and hence equate to a limiting case of a Gaussian operator from Eq (4.23) above.

Next, define a squeezed off-diagonal Gaussian in terms of the thermal case, which we have already proved has a positive representation:

$$
\tilde{\Lambda}^{(s)}(\mu(\epsilon), \xi(\epsilon), \nu') = \prod_{i > j} \left[1 - \xi_{ij} \hat{b}_i \hat{b}_j\right] \tilde{\Lambda}[\mu(\epsilon), \nu'] .
$$

(4.25)

where:

$$
\xi_{ij}(\epsilon) = \sum_{\{i', j'\} \in \bar{\sigma}} \frac{\delta_{i'i'} \delta_{j'j}}{-\epsilon} .
$$

(4.26)

Next, consider the limit of $\epsilon \to 0$ as before, so that to leading order,

$$
\hat{\rho}_{\vec{n} \vec{m}'} = : \prod_{\{i, j\} \in \sigma} \left[\hat{a}_i \hat{a}_j\right] |\vec{n}'\rangle \langle \vec{n}'| :
$$

$$
= \lim_{\epsilon \to 0} \epsilon^{S + \delta M} \tilde{\Lambda}^{(s)}[\mu(\epsilon), \xi(\epsilon), \vec{n}'] .
$$

(4.27)

A positive expansion parameter is obtained here as well, thus completing the proof.
D. Differential Properties

We can differentiate the Gaussian operators with respect to their parameters to get

\[
\frac{d}{d\Omega} \hat{\Lambda} = \frac{1}{\Omega} \hat{\Lambda},
\]

\[
\frac{d}{d\sigma} \hat{\Lambda} = \sigma^{-1} \hat{\Lambda} - \sigma^{-1} \hat{b} \hat{b}^\dagger \hat{\Lambda} : \sigma^{-1},
\]

(4.28)

where the matrix derivative is defined as

\[
\left( \frac{\partial}{\partial \sigma} \right)_{\mu,\nu} = \frac{\partial}{\partial \sigma_{\mu\nu}},
\]

(4.29)

i.e. involving a transpose. These expressions for the derivative can be inverted to obtain the important identities:

\[
\hat{\Lambda} = \Omega \frac{\partial}{\partial \Omega} \hat{\Lambda},
\]

\[
\hat{b} \hat{b}^\dagger \hat{\Lambda} : = \sigma \hat{\Lambda} - \sigma \frac{\partial \hat{\Lambda}}{\partial \sigma} \sigma,
\]

(4.30)

and thus we can write the normally ordered action of any pair of operators on a Gaussian as a derivative. As theorems 5 and 6 in Appendix B show, there are analogous identities for antinormally ordered and mixed pairs:

\[
\{ \hat{b} : \hat{\Lambda} \} = -\sigma \hat{\Lambda} + (\sigma - I) \frac{\partial \hat{\Lambda}}{\partial \sigma},
\]

\[
\{ \hat{b} b^\dagger \hat{\Lambda} \} = (\sigma - I) \hat{\Lambda} - (\sigma - I) \frac{\partial \hat{\Lambda}}{\partial \sigma} (\sigma - I) .
\]

(4.31)

For the subset of Gaussian operators that correspond to (generalised) thermal states, i.e. \( m^+ = m = 0 \), we obtain a simpler set of differential identities:

\[
\hat{b}^T \hat{b}^T \hat{\Lambda} = n \hat{\Lambda} + (I - n) \frac{\partial \hat{\Lambda}}{\partial m} n,
\]

\[
\hat{\Lambda} \hat{b}^T \hat{b}^T = n \hat{\Lambda} + n \frac{\partial \hat{\Lambda}}{\partial m} (I - n),
\]

\[
\hat{b}^T \hat{b} \hat{\Lambda} = (I - n) \hat{\Lambda} + (I - n) \frac{\partial \hat{\Lambda}}{\partial m} (I - n),
\]

\[
\left( \hat{b} b^\dagger \right)^T = n \hat{\Lambda} - n \frac{\partial \hat{\Lambda}}{\partial m} n .
\]

(4.32)

V. GAUSSIAN REPRESENTATION

The completeness and positivity of the basis formed from the Gaussian operators allows us to expand the density operator for any physical state \( \hat{\rho}(t) \) as:

\[
\hat{\rho}(t) = \sum_i P_i(t) \hat{\Lambda}(\lambda_i),
\]

\[
= \int P(\lambda, t) \hat{\Lambda}(\lambda)d\lambda ,
\]

(5.1)

where the expansion coefficients are normalised to one \( \int P(\lambda, t)d\lambda = 1 \). This expansion defines a type of phase-space representation of the state: the vector \( \lambda \) of Gaussian parameters becomes a generalised phase-space coordinate, the function \( P(\lambda, t) \) is then a probability distribution function over the generalised phase space, and \( d\lambda = d^{2(p+1)} \) is the phase-space integration measure.

A. Moments

Some basic properties of \( P(\lambda, t) \) follow from those of the Gaussian operators. For example, using the trace result of Eq. (4.30), we find

\[
\text{Tr} [\hat{\rho}] = \int P(\lambda, t)d\lambda \equiv \Omega .
\]

(5.2)

Thus the normalised distribution \( \Omega(\lambda) \) can represent unnormalised density operators by incorporating the normalisation into the mean weight \( \Omega \).

More generally, the expectation values of an operator \( \hat{O} \) evaluate to

\[
\langle \hat{O} \rangle = \text{Tr} [\hat{O} \hat{\rho}] / \text{Tr} [\hat{\rho}] = \int P(\lambda, t) \hat{\Lambda} \hat{O} d\lambda / \Omega
\]

\[
= \text{Tr} [\hat{O} \hat{\Lambda}] / \Omega
\]

\[
= \langle O(\lambda) \rangle_p ,
\]

(5.3)

where the phase-space function \( O(\lambda) \) corresponding to the operator \( \hat{O} \) is

\[
O(\lambda) \equiv \text{Tr} \left( \hat{O} \text{Pf} \left[ \sigma^{-1} \right] : \text{exp} \left[ \hat{b}^\dagger (I - \sigma^{-1}/2) \hat{b} \right] : \right).
\]

(5.4)

Physical quantities thus correspond to (weighted) moments of \( P \). For example, from Eq. (5.4), we find that the normal and anomalous averages of the state correspond to first order moments:

\[
\langle \hat{b}_i \hat{b}_j \rangle = \langle n_{ij} \rangle_p ,
\]

\[
\langle \hat{b}_i \hat{b}_j \rangle = \langle n_{ij} \rangle_p ,
\]

\[
\langle \hat{b}_i \hat{b}_j \rangle = \langle m_{ij}^+ \rangle_p ,
\]

(5.5)

and normally ordered number-number correlations correspond to second-order moments:

\[
\langle : \hat{n}_i \hat{n}_j : \rangle = \langle n_{ij} n_{ji} - n_{ij} n_{ji} - m_{ij} m_{ji}^+ \rangle_p ,
\]

(5.6)
where \( \hat{n}_i \equiv \hat{b}_i^\dagger \hat{b}_i \).

Similarly, higher-order correlations correspond to higher-order moments, the form of which is determined by evaluation of the Gaussian trace Eq. \( \text{(5.4)} \). One way to do this is to use the moment generating function derived in Theorem 3 of Appendix \[19\].

We note that the expectation value of any odd product of operators must vanish e.g. \( \langle \hat{b}_i \rangle = 0 \). Thus the distribution cannot represent any superposition of states whose total number differ by an odd number. Such superposition states we exclude from our definition of physical state, as they are not generated by evolution under any known physical Hamiltonian. The Gaussian distribution can, however, represent systems in which particles are coherently added or removed in pairs, leading to nonzero anomalous correlations \( \langle m_{ij} \rangle \). On the other hand, if the total number of particles is conserved or changed only via contact with a Markovian reservoir, then the anomalous correlations will be identically zero and we can represent the system via an expansion in only the thermal subset of Gaussian operators.

\[ \text{B. Time evolution} \]

The (real or imaginary) time evolution of a density operator is determined by a master equation, of the general form

\[
\frac{d}{dt} \hat{\rho}(t) = \hat{L}[\hat{\rho}(t)],
\]

where the \( \hat{L} \) is a superoperator that pre- and post-multiplies the density operator by combinations of annihilation and creation operators. For Hamiltonian dynamics, the superoperator is a commutator with the Hamiltonian: \( \hat{L}[\hat{\rho}] = -i/\hbar [\hat{H}, \hat{\rho}] \). For an open quantum system, there will be additional terms, of the Lindblad form, to describe the coupling to the environment \[19\]. To calculate the equilibrium state at temperature \( T = 1/k_B \tau \), one can solve an ‘imaginary time’ equation for the normalised density operator: \( d\hat{\rho}/dT = -\frac{1}{\tau} [\hat{H} - \mu N, \hat{\rho}]_+ \).

To determine the time evolution of the distribution corresponding to Eq. \( \text{(5.6)} \), we first substitute for \( \hat{\rho} \) the expansion in Eq. \( \text{(5.11)} \):

\[
\int \frac{dP(\hat{\lambda}, t)}{dt} \hat{\Lambda}(\hat{\lambda}) d\hat{\lambda} = \int P(\hat{\lambda}, t) \hat{L}[\hat{\Lambda}(\hat{\lambda})] d\hat{\lambda}.
\]

Second, we use the differential identities in Eqs. \[18\] to convert the superoperator \( \hat{L}[\hat{\lambda}] \) into an operator \( \hat{L}[\hat{\lambda}] \) that contains only derivatives of \( \hat{\lambda} \). Next we integrate by parts to obtain, provided that no boundary terms arise,

\[
\frac{d}{dt} P(\hat{\lambda}, t) = \int L'[P(\hat{\lambda}, t)] \hat{\Lambda}(\hat{\lambda}) d\hat{\lambda},
\]

where \( L' \) is a reordered form of \( L \), with a sign change to derivatives of odd order. Finally, we see that this equation holds if the distribution function satisfies the evolution equation

\[
\frac{d}{dt} P(\hat{\lambda}, t) = L'[P(\hat{\lambda}, t)].
\]

This procedure for going from the master equation for \( \hat{\rho} \) to the evolution equation for \( P \) can be summarised as a set of operator correspondences:

\[
\hat{b}^\dagger \hat{b}^\dagger \hat{\rho} \rightarrow \left[ \sigma + \left\{ \frac{\partial}{\partial \sigma^T} \sigma \right\}^T \right] P,
\]

\[
\hat{b} \hat{b}^\dagger \hat{\rho} \rightarrow \left[ \sigma - \left\{ \frac{\partial}{\partial \sigma^T} (\sigma - I)^T \right\} \right] P,
\]

\[
\left( \hat{b}^\dagger \hat{b}^\dagger \hat{\rho} \right)^T \rightarrow \left[ \sigma - I + \left\{ \frac{\partial}{\partial \sigma^T} (\sigma - I)^T \right\} (\sigma - I) \right] P.
\]

Alternatively, for a system in which the total number is conserved, we can use these thermal correspondences:

\[
\hat{b}^T \hat{b}^T \hat{\rho} \rightarrow \left[ n - \left\{ \frac{\partial}{\partial n^T} (I - n^T) \right\}^T n \right] P,
\]

\[
\hat{b} \hat{b}^T \hat{\rho} \rightarrow \left[ n - \left\{ \frac{\partial}{\partial n^T} (I - n^T) \right\} (I - n) \right] P,
\]

\[
\left( \hat{b}^T \hat{b}^T \hat{\rho} \right)^T \rightarrow \left[ n + \left\{ \frac{\partial}{\partial n^T} (I - n^T) \right\} n \right] P.
\]

To be able to sample the time evolution of \( P \) with stochastic phase-space equations, which is the final goal, we must have an evolution equation that is in the form of a Fokker-Planck equation, containing first and second order derivatives:

\[
\frac{d}{dt} P(\hat{\lambda}, t) = \left[ \frac{1}{2} \sum_{j,k=0}^p \frac{\partial}{\partial \lambda_j} \frac{\partial}{\partial \lambda_k} D_{j,k}(\hat{\lambda}) - \sum_{j=0}^p \frac{\partial}{\partial \lambda_j} A_j(\hat{\lambda}) \right] P(\hat{\lambda}, t),
\]

\[\text{(5.12)}\]
where the matrix $D_{j,k}$ must be positive-definite (when the Fokker-Planck equation is written in terms of real variables). A Monte-Carlo type sampling of Eq. (5.11) can be realised by integrating the Ito stochastic equations

$$d\lambda_j(t) = A_j(\lambda)\,dt + \sum_l B_{j,l}(\lambda)\,dW_l(t) , \quad (5.13)$$

where $dW_l(t)$ are Weiner increments, obeying $\langle dW_l(t)\,dW_l(t') \rangle = \delta_{l,l'}\delta(t-t')dt$, i.e. Gaussian white noise. The noise matrix $B_{j,l}$ is related to the diffusion matrix by $D_{j,k} = \sum_l B_{j,l}B_{k,l}$.

The final phase-space equations are far from being unique. This freedom in the final form arises from different choices that are made at different points in the procedure. The choices at some points are constrained by the need to generate genuine Fokker-Planck equation. Other points, the choices are in principle free; they affect the final stochastic behaviour without changing observable moments. They are thus a stochastic analogue of a gauge choice in field theories. A good choice of stochastic gauge can dramatically improve the signal-to-noise ratio in simulations. We defer a full discussion of stochastic gauges to another place, where they will be illustrated by application in practical examples. However we note that because the Gaussian basis is analytic, methods previously used for the (bosonic) stochastic gauge positive-P representation are therefore applicable. Furthermore, for fermionic systems there is an additional freedom in the choice of operator correspondences, arising from vanishing operator products. Such a fermionic stochastic gauge was instrumental in overcoming the sign problem in the Hubbard simulations.

1. Evolution of a free gas

Hamiltonians that are only quadratic in the Fermi ladder operators, such as that of a noninteracting gas, will map to a Fokker-Planck equation that contains only first order derivatives. The evolving quantum state can thus be sampled by a single, deterministic trajectory. As an example of this consider the equilibrium calculation of a gas of noninteracting particles. The governing Hamiltonian is always diagonalizable, and can be written as:

$$\hat{H} = \hbar \hat{b}^\dagger \omega \hat{b} , \quad (5.14)$$

where $\omega_{i,j} = \delta_{i,j}\omega_j$ are the single-particle energies. The canonical distribution at temperature $T = 1/k_B\tau$ is found from the equation

$$\hbar \frac{\partial}{\partial \tau} \hat{\rho} = \frac{\hbar}{2} \left( \hat{b}^\dagger \omega \hat{b} \hat{\rho} + \hat{\rho} \hat{b}^\dagger \omega \hat{b} \right) . \quad (5.15)$$

Applying the thermal correspondences in Eq. (5.11), we obtain the the Fokker-Planck equation

$$\frac{\partial P}{\partial \tau} = \sum_k \omega_k \left[ \frac{\partial}{\partial n_k} (1 - n_k) + \frac{\partial}{\partial \Omega} \Omega \right] n_k P . \quad (5.16)$$

This Fokker-Planck equation with first-order derivatives corresponds to deterministic characteristic equations:

$$\dot{\Omega} = -\sum_k \omega_k \Omega n_k , \quad (5.17)$$

$$\dot{n}_k = -\omega_k n_k (1-n_k) . \quad (5.18)$$

Integrating the deterministic equation for the mode occupation $n_k$ leads to the usual Fermi-Dirac distribution:

$$n_k = \frac{1}{e^{\omega_k \tau} + 1} . \quad (5.19)$$

The weighting term occurs because this method of obtaining a thermal density matrix results in an unnormalized density matrix with trace equal to $\Omega(\tau)$. From integration of the above equation one finds that

$$\text{Tr} [\hat{\rho}_u] = \Omega(\tau) = \Omega_0 \Pi_k e^{-\omega_k n_k \tau} , \quad (5.20)$$

i.e. the weight decays exponentially, at a rate given by the total energy.

VI. CONCLUSION

The operator representations introduced here represent the largest class of fermionic representations that can be constructed using an operator basis that is Gaussian in the elementary annihilation and creation operators, excluding ‘odd’ forms that would require Grassmann algebra. The operator representations are able to represent arbitrary physical states of fermions, in which there are no coherences between states whose total number differs by an odd number.

Furthermore, the overcompleteness of the Gaussian basis makes it possible to express any physical density operator as a probabilistic distribution over the Gaussian operators. We have derived the identities which are essential for first-principles calculations of the time evolution of quantum systems, both dynamical (real time) and canonical (imaginary time). Interacting Hamiltonians, containing terms that are up to fourth order in ladder operators, can be solved by use of stochastic sampling methods, since they can be transformed into a second-order Fokker-Planck equation, provided a suitable stochastic gauge is chosen to ensure that the distribution remains sufficiently bounded.

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Appendix A: GRASSMANN ALGEBRA

This appendix introduces the basic concepts of non-commuting algebra and lists some results pertaining to Grassmann calculus and Fermi coherent states. These results are used in Appendix B to establish the properties of the Gaussian operators. Proofs and further discussion of these results can be found in the literature [15, 23, 24].

Let \( \mathbf{a} \) be a vector of \( M \) anticommuting (Grassmann) numbers, i.e.

\[
[\alpha_i, \alpha_j]_+ = 0 .
\]

(A1)

Since \( \alpha_i^2 = 0 \), any function of Grassmann numbers can be at most linear in any one of its arguments. Thus, for example, the single mode exponential is

\[
\exp(\alpha_j) = 1 + \alpha_j ,
\]

(A2)

and a multimode exponential, e. g. \( \exp(\sum \alpha_j) \) will be an ordered product of such single-mode exponentials. The Grassmann numbers must anticommute with all Fermi annihilation and creation operators.

1. Grassmann Calculus

Differentiation of a single Grassmann variable is defined as

\[
\frac{\partial}{\partial \alpha_i} \alpha_j = \delta_{ij} ,
\]

(A3)

with the derivative of products obtained by the Grassmann chain rule:

\[
\frac{\partial}{\partial \alpha_j} [f(\alpha)g(\alpha)] = \begin{cases} \frac{\partial f}{\partial \alpha_j} g + f \frac{\partial g}{\partial \alpha_j} , & f \text{ even} \\ \frac{\partial f}{\partial \alpha_j} g - f \frac{\partial g}{\partial \alpha_j} , & f \text{ odd} \end{cases}
\]

(A4)

i. e. the derivative operator also anticommutes.

Grassmann integration is defined to be the same as differentiation, but written in a different way:

\[
\int d\alpha_j = 0
\]

\[
\int \alpha_j d\alpha_j = 1 .
\]

(A5)

Multivariate integrals are ordered sequences of single-variable integrations, which can be written without ambiguity if the integration measure (as for a derivative) is also taken to be an anticommuting number. For an integral over all variables in a vector, we define the integration measure to be ordered in increasing numerical order: \( d\mathbf{a} \equiv d\alpha_1...d\alpha_N \).

Note that integrating a total derivative gives zero:

\[
\int d\alpha_j \frac{\partial}{\partial \alpha_j} f = 0 .
\]

(A6)

This fact, coupled with the product rule, gives a result for partial integration:

\[
\int d\alpha_j \frac{\partial f}{\partial \alpha_j} g = \begin{cases} -\int d\alpha_j f \frac{\partial g}{\partial \alpha_j} , & f \text{ even} \\ \int d\alpha_j f \frac{\partial g}{\partial \alpha_j} , & f \text{ odd} \end{cases} .
\]

(A7)

One very useful result is the multivariate Gaussian integral:

\[
\int \exp(-\mathbf{a}^T \mathbf{A} \mathbf{a}/2) d\mathbf{a} = \text{Pf} [\mathbf{A}]^M
\]

for an antisymmetric matrix \( \mathbf{A} \) of complex numbers. The Pfaffian is related to the determinant \( (\text{Pf} [\mathbf{A}])^2 = \det \mathbf{A} \), and thus, apart from a sign change, has many of the same properties. For example, \( \text{Pf} [\mathbf{A}^T] = (-1)^N \text{Pf} [\mathbf{A}] \) and \( |\text{Pf} [\mathbf{A}^{-1}]| = |1/\text{Pf} [\mathbf{A}]| \). Another useful type of Gaussian integral is:

\[
\int \exp(-\mathbf{B} \mathbf{a}) \prod d\beta_j \prod \alpha_j = \det [\mathbf{B}]^M
\]

where \( \mathbf{B} \) is a square matrix of complex numbers and \( \beta \) and \( \alpha \) are two independent Grassmann variables. This second integral is in fact a special case of the first, except with \( 2M \) total Grassmann variables.

2. Grassmann coherent states

For each Grassmann number \( \alpha_j \) we can associate another Grassmann number, denoted \( \bar{\alpha}_j \), to play the role of a complex conjugate. This is formally regarded as an independent variable for calculus purposes. The conjugates \( \bar{\alpha}_j \) anticommute with all other Grassmann variables. By use of such a complex Grassmann algebra, we can define a fermionic coherent state, which is formally an eigenstate of the annihilation operator:

\[
|\alpha_j\rangle = (1 + \bar{\alpha}_j \alpha_j)^{-\frac{1}{2}} (|0\rangle + |1\rangle \alpha_j)
\]

(A10)

\[
\langle \alpha_j\rangle = (1 + \bar{\alpha}_j \alpha_j)^{-\frac{1}{2}} (|0\rangle + \bar{\alpha}_j (|1\rangle)
\]

(A11)

Like the bosonic coherent state, the fermionic coherent state can be written as (Grassmann) displacement from the vacuum:

\[
|\alpha_j\rangle = \exp (\bar{\alpha}_j \alpha_j - \bar{\alpha}_j \alpha_j) |0\rangle
\]

(A12)

Multimode coherent states are products of the single-mode states:

\[
|\alpha\rangle = \prod_{j=1}^M |\alpha_j\rangle
\]

\[
= \exp \left[ \left( \sum_{j=1}^M \bar{\alpha}_j \alpha_j - \bar{\alpha}_j \alpha_j \right) \right] |0\rangle
\]
The inner product of two states is:
\[ \langle \alpha_i | \alpha_j \rangle = \exp(\overline{\alpha}_i \alpha_j - \overline{\alpha}_i \alpha_j/2 - \overline{\alpha}_j \alpha_j/2) , \] (A13)
and thus as two special cases:
\[ \langle \alpha_i | \alpha_i \rangle = 1 \]
\[ \langle -\alpha_i | \alpha_i \rangle = \exp(-2\overline{\alpha}_i \alpha_i) . \] (A14)

The usefulness of the coherent states lies in the fact that they form a complete set:
\[ \int d\alpha_j |\alpha_j \rangle \langle \alpha_j | = |0\rangle \langle 0| + |1\rangle \langle 1| = I \] , (A15)
or, for the multimode case,
\[ \int d\alpha |\alpha \rangle \langle \alpha | = I_M , \] (A16)
where we have defined a 2M-variate integration measure as
\[ d\alpha = \prod_{j=1}^{M} (d\overline{\alpha}_j d\alpha_j) . \] (A17)

Finally, we can express the trace of an arbitrary operator \( \hat{O} \) as
\[ \text{Tr} [\hat{O}] = \int d\alpha \langle -\alpha | \hat{O} |\alpha \rangle . \] (A18)

**Appendix B: GAUSSIAN FERMION OPERATORS**

We prove some useful results concerning the most general multi-mode Gaussian operator constructed from fermionic ladder operators. The proofs make use of the properties of Grassmann coherent states and anticommuting algebra, which are summarized in Appendix A.

However the final results do not contain any Grassmann variables. The results establish the properties of the Gaussian operators that are discussed in Sec. IV. In particular, they enable the phase-space representation for fermions introduced in Sec. IV.

1. General Gaussian Operator

In this appendix, we use the vector and ordering notations introduced in Sec. III. We find it convenient to define an unnormalised Gaussian form of Fermi operators:
\[ \hat{\Lambda}^{(u)} (\underline{\alpha}) = : \exp \left[ -\frac{1}{2} \frac{c^\dagger}{\overline{\alpha}} \Lambda \frac{c}{\overline{\alpha}} \right] : \\
\equiv \sum_{n=0}^{\infty} \frac{1}{2^n n!} : \frac{c^\dagger}{\overline{\alpha}} \Lambda \frac{c}{\overline{\alpha}} \right)^n : \\
= \sum_{\mu, \nu = 1}^{2M} \left( 1 - \frac{1}{2} \frac{c^\dagger}{\overline{\alpha}} \Lambda_{\mu \nu} \frac{c}{\overline{\alpha}} \right) : , \] (B1)

where \( \underline{\alpha} \) is a \( 2M \times 2M \) matrix of parameters. Note that this Gaussian form contains no displacements (offsets), as this would mean that products containing odd numbers of ladder operators would appear in the Taylor series expansion. These we exclude as surplus structure, on the physical grounds that they do not appear in any known observable or Hamiltonian. In terms of the covariance matrix \( \underline{\sigma} \), the unnormalised Gaussian is:
\[ \hat{\Lambda}^{(u)} (\underline{\sigma}) = : \exp \left[ \frac{c^\dagger}{\overline{\alpha}} (\frac{1}{2} \underline{\sigma}^{-1} / 2) \frac{c}{\overline{\alpha}} \right] : , \] (B2)

where the relation between the two parametrizations is \( \underline{\sigma} = [\Lambda + 2I]^{-1} \) and where the diagonal matrix \( I \) is as defined in Eq. (B4).

Because of the anticommuting property of fermions, both \( \underline{\alpha} \) and \( \underline{\Lambda} \) possess a generalized antisymmetry: \( \underline{\alpha} = -\underline{\alpha}^T \), \( \underline{\Lambda} = -\underline{\Lambda}^T \), or more in block matrix form,
\[ \begin{bmatrix} a & b \\ c & d \end{bmatrix} = -X \begin{bmatrix} a & b \\ c & d \end{bmatrix}^T \]
\[ = - \begin{bmatrix} d^T & b^T \\ c^T & a^T \end{bmatrix} , \] (B3)

where the constant matrix \( X \) is defined as
\[ X = \begin{bmatrix} 0 & I \\ I & 0 \end{bmatrix} . \] (B4)

When applied to the left of a matrix, \( X \) swaps the upper and lower halves; when applied to the right, it swaps the left and right halves. This structure means that the matrices \( \underline{\alpha} \) and \( \underline{\Lambda} \) can be transformed into explicitly antisymmetric forms by certain permutations of rows and columns. For example, it follows immediately from Eq. (B3) that interchanging left and right halves, or upper and lower halves, will generate an antisymmetric matrix. Alternatively, inserting each row in the lower half after the corresponding row in the upper half, and inserting each column in the right half before the corresponding row in the left half generates the antisymmetric form
\[ \begin{bmatrix} a & b \\ c & d \end{bmatrix} \equiv \begin{bmatrix} b_{11} & a_{11} & \cdots & b_{1M} & a_{1M} \\ d_{11} & c_{11} & \cdots & d_{1M} & c_{1M} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ b_{M1} & a_{M1} & \cdots & b_{MM} & a_{MM} \\ d_{M1} & c_{M1} & \cdots & d_{MM} & c_{MM} \end{bmatrix} \] (B5)

With the covariance matrix antisymmetrized in this way, the Gaussian operator becomes
\[ \hat{\Lambda}^{(u)} (\underline{\sigma}_A) = : \exp \left[ \frac{c^\dagger}{\overline{\alpha}_A} (\frac{1}{2} \underline{\sigma}_A^{-1} / 2) \frac{c}{\overline{\alpha}_A} \right] : , \] (B6)
where the vector of operators is now
\[
\hat{\Lambda}_A = \begin{pmatrix}
\hat{b}_1 \\
\hat{b}_1^* \\
\vdots \\
\hat{b}_M \\
\hat{b}_M^*
\end{pmatrix}.
\]  (B7)

The generalised antisymmetry of \( \alpha \) and \( \lambda \) has implications for matrix derivatives. Because each element of the matrix appears twice, we have \( \partial \sigma_{\mu\nu}/\partial \sigma_{\nu\mu} = \delta_{\mu\nu} \), where \( \delta_{\mu\nu} \) is the Kronecker delta function. The extra terms here appear in the derivative of an inverse:
\[
\frac{\partial \sigma_{\mu\nu}^{-1}}{\partial \sigma_{\nu\mu}} = \sigma_{\mu\mu}^{-1} \sigma_{\nu\nu}^{-1} + \sigma_{\mu\nu}^{-1} X_{\gamma\phi} X_{\theta\epsilon} \sigma_{\epsilon\nu}^{-1},
\]  (B8)
and they also give an additional factor of two in the derivative of a determinant:
\[
\frac{d}{d\alpha} \sqrt{\det \sigma} = \sqrt{\det \sigma^{-1}},
\]  (B9)
where we define the matrix derivative as
\[
\left( \frac{d}{d\alpha} \right)_{\mu\nu} = \frac{d}{d\sigma_{\mu\nu}},
\]  (B10)
i.e. involving a transpose. The result (B8) allows us to relate the derivatives with respect to \( \sigma \) and \( \lambda \):
\[
\frac{df}{d\lambda} = \frac{df}{d\alpha} \sigma^{-1} - \sigma \frac{df}{d\sigma} \sigma^{-1}.
\]  (B11)

2. Normalisation

**Theorem 1:** The trace of the unnormalised Gaussian operator is equal to the Pfaffian of the inverse of the antisymmetrized covariance, i.e.
\[
N \equiv \text{Tr} \left[ \Lambda^{(u)} | \sigma \right] = \text{Pf} \left[ \sigma_A^{-1} \right],
\]  (B12)
where Pf stands for Pfaffian.

**Proof:** Because the Gaussian is in normally ordered form, it is straightforward to evaluate the trace with multimode Grassmann coherent states \( | \alpha \rangle \), using the Grassmann trace result of Eq. (A18):
\[
\text{Tr} \left[ \Lambda^{(u)} \right] = \int \langle -\alpha | \Lambda^{(u)} | \alpha \rangle \prod_j [d\alpha_j d\sigma_j]
= \int \exp \left[ -\alpha^\dagger \sigma^{-1} \alpha / 2 \right] \prod_j [-d\sigma_j d\alpha_j],
\]  (B13)
where we have made use of the fact that, from the Grassmann inner product result of Eq. (A16), \( \langle -\alpha | \alpha \rangle = \text{exp}(-2\sigma_\alpha) \). We have also changed variables: \( \alpha_j \rightarrow -\sigma_j \), and introduced 2M-vectors of Grassmann variables \( \alpha \equiv (\alpha, \sigma, \alpha^T)^T \) and \( \sigma_A \equiv (\alpha, \sigma^T)^T \). Changing to the antisymmetric form of the covariance \( \sigma_A^{-1} \) and swapping the order of the pairs in the integration measure, we obtain
\[
\text{Tr} \left[ \Lambda^{(u)} \right] = \int \exp \left[ -\alpha^T \sigma_A^{-1} \alpha / 2 \right] \prod_j [d\alpha_j d\sigma_j],
\]  (B14)
where the reordered Grassmann vector is \( \alpha_A \equiv (\alpha_1, \sigma_1, ..., \alpha_M, \sigma_M)^T \). Noting that the arrangement of elements in \( \alpha_A \) matches the order of integration, we can apply the Gaussian integral result [Eq. (A8)]:
\[
\text{Tr} \left[ \Lambda^{(u)} \right] = \text{Pf} \left[ \sigma_A^{-1} \right].
\]  (B15)
QED.

**Corollaries:**

Now the square of the Pfaffian of a matrix is equal to its determinant. Thus, to within a \( \pm \) sign, the normalisation is determined by the determinant of the covariance:
\[
\left( \text{Tr} \left[ \Lambda^{(u)} \right] \right)^2 = \frac{1}{\text{det} \left[ \sigma_A \right]} = (-1)^M \frac{1}{\text{det} \left[ i\sigma \right]} = \frac{1}{\text{det} \left[ i\sigma_A \right]},
\]  (B16)
and thus we may write the Gaussian operator in normalised form as
\[
\hat{\Lambda} = \pm \sqrt{\text{det} \left[ i\sigma_A \right]} : \exp \left[ \hat{b}^\dagger (\frac{1}{2} - \frac{1}{2} \sigma^{-1} \hat{b}) \right] :.
\]  (B17)

where the choice of plus/minus sign is determined by \( \sqrt{\text{det} \left[ i\sigma_A \right]} \) Pf \( \left[ \sigma_A^{-1} \right] \). This extra sign, or phase, which does not appear in the normalizations of the familiar complex-number or bosonic Gaussians, fortunately does not appear in any of the identities needed to make use of the Gaussian operators as a basis for a phase-space representation.

A specific case where the determinant appears is for the generalised thermal Gaussian without squeezing parameters, so that \( m = m^* = 0 \). In this case, the normalisation follows directly from the second Grassmann Gaussian integral identity, Eq. (A20). Following the same procedure as before, we find that:
\[
\text{Tr} \left[ \Lambda^{(u)} \right] = \text{det} \left[ 2I - \lambda \right].
\]  (B18)

3. Second-order moments
Theorem 2: The fermionic Gaussian operator is completely characterised by its second-order moments. In particular, the covariance matrix corresponds to the second-order moments in normally ordered trace form, i.e.

\[
\text{Tr} \left[ \hat{b} \hat{b}^\dagger \hat{A} \right] = \sigma_{bb}, \quad (B19)
\]

where \( \hat{b} \hat{b}^\dagger \) is a matrix multiplication of two vectors, resulting in the \( 2M \times 2M \) matrix of Eq. (B2). Proof: We proceed as in the proof of Theorem 1, by taking the trace of the unnormalised form using Grassmann coherent states and then changing variables: \( \pi_j \rightarrow -\pi_j \): \n
\[
\text{Tr} \left[ \hat{b} \hat{b}^\dagger \hat{A}^{(u)} \right] = \int \left\langle -\alpha | \hat{b} \hat{b}^\dagger \hat{A}^{(u)} | \alpha \right\rangle \prod_j [d\pi_j d\alpha_j]
\]

\[
= \int \alpha \alpha^\dagger \exp \left\{ -\frac{\alpha^\dagger \sigma^{-1} \alpha}{2} \right\} \prod_j [d\alpha_j d\bar{\alpha}_j].
\]

(B20)

Next we put the integral into the form Eq. (A8): \n
\[
\text{Tr} \left[ \hat{b} \hat{b}^\dagger \hat{A}^{(u)} \right] = \int \left\langle O \right| \hat{b} \hat{b}^\dagger \hat{A}^{(u)} = \prod_j [d\alpha_j d\bar{\alpha}_j]
\]

\[
= \frac{d}{da^{-1}} \int \exp \left\{ -\frac{\alpha^\dagger \sigma^{-1} \alpha}{2} \right\} \prod_j [d\alpha_j d\bar{\alpha}_j] , \quad (B21)
\]

where in taking the derivative with respect to \( \sigma^{-1} \) we have taken account of the fact that each element of it appears twice, owing to its generalized antisymmetry. Evaluating the Grassmann integral, and employing the determinant result, we get

\[
\text{Tr} \left[ \hat{b} \hat{b}^\dagger \hat{A}^{(u)} \right] = \frac{d}{da^{-1}} (\pm) \sqrt{\det [i\sigma^{-1}]}
\]

\[
= \pm \sqrt{\det [i\sigma^{-1}]} a. \quad (B22)
\]

Finally, dividing through by the normalisation in Eq. (B12) gives the normalised result. QED.

Corollaries:

We can put Eq. (B19) into a more familiar form by using the cyclic property of trace:

\[
\text{Tr} \left[ \hat{b} \hat{b}^\dagger \hat{A} \right] = \text{Tr} \left[ -\left( \hat{b}^T \hat{A} \hat{b}^T \right) \right] = \text{Tr} \left[ \hat{b}^T \hat{b}^\dagger \hat{A} \right] = \text{Tr} \left[ \hat{b}^T \hat{b}^\dagger \hat{A} \right]
\]

\[
= \left[ \begin{array}{c}
n^T - I \\
\text{m}^+ - I - n
\end{array} \right] \hat{A}, \quad (B23)
\]

where we have defined the matrix \( n \) for the number, or normal, moments, and the matrices \( \text{m} \) and \( \text{m}^+ \) for the squeezing, or anomalous, moments, as follows:

\[
n = \left\langle \hat{b}^T \hat{b}^T \right\rangle_{\hat{A}}, \quad \text{m} = \left\langle \hat{b} \hat{b}^T \right\rangle_{\hat{A}}, \quad \text{m}^+ = \left\langle \hat{b}^T \hat{b} \right\rangle_{\hat{A}}, \quad (B24)
\]

where \( \langle \hat{O} \rangle_{\hat{A}} = \text{Tr} \left[ \hat{O} \hat{A} \right] \). Thus we can write covariance matrix in terms of the moments as

\[
\sigma = \left[ \begin{array}{c}
n^T - I \\
\text{m}^+ - I - n
\end{array} \right], \quad (B25)
\]

or inverting the relationship,

\[
\left\langle \hat{b} \hat{b}^\dagger \right\rangle_{\hat{A}} = I - I \sigma I. \quad (B26)
\]

4. Higher-order moments

One can calculate higher-order moments along similar lines, i.e. by expanding the trace as a Grassmann integral then converting this into a higher-order derivative of a determinant. The results of this procedure in the general case can be written in terms of a moment generating function.

Theorem 3: Any even moment of a Gaussian operator, in normally ordered trace form, can be calculated by means of the moment generating function

\[
M(\tau) \equiv \sqrt{\det [\tau^2 - \sigma]} \quad (B27)
\]

as follows

\[
\text{Tr} \left[ \hat{b}^\dagger_{\mu_1} \hat{b}_{\mu_2} \cdots \hat{b}^\dagger_{\mu_r} \hat{b}_{\mu_r} \hat{A} \right] = \frac{\partial}{\partial \tau_{\mu_1,\mu_2}} \cdots \frac{\partial}{\partial \tau_{\mu_{r-1},\mu_r}} M(\tau) \Bigg|_{\tau=0} \quad (B28)
\]

Proof: We start by writing the normally ordered operator product as a derivative of a normally ordered Gaussian:

\[
\hat{b}^\dagger_{\mu_1} \hat{b}_{\mu_2} \cdots \hat{b}^\dagger_{\mu_r} \hat{b}_{\mu_r} = \frac{\partial}{\partial \tau_{\mu_1,\mu_2}} \cdots \frac{\partial}{\partial \tau_{\mu_{r-1},\mu_r}} \exp \left[ \hat{b}^\dagger \tau \hat{b}/2 \right] \Bigg|_{\tau=0} \quad (B29)
\]

where \( \tau \) is a \( 2M \times 2M \) matrix of complex numbers with the generalised antisymmetry \( \tau = -\tau^\dagger \). Using this result
Thus the normally ordered triple correlations are:
\[
\text{Tr} \left[ \hat{n}_i \hat{n}_j \hat{n}_k : \hat{\Lambda} \right] = n_{ij} n_{jk} n_{ki} - n_{ij} \left( n_{jk} n_{kj} + m_{jk} m_{kj}^+ \right) + n_{ij} n_{jk} n_{kj} - n_{ij} \left( n_{kj} n_{ki} + m_{kj} m_{ki}^+ \right) + n_{ij} n_{kj} n_{ik} - n_{ik} \left( n_{ij} n_{ji} + m_{ij} m_{ji}^+ \right) + n_{ij} n_{ik} m_{ik}^+ + n_{ij} m_{ik} m_{ik}^+ + n_{ikj} m_{ij}^+ + n_{ik} m_{kj} m_{ij}^+, \tag{B37}
\]
again as expected for a state with Gaussian correlations.

5. Normally ordered products

**Theorem 4:** A normally ordered product of a pair of ladder operators and a Gaussian is equivalent to a first-order differential operator on the Gaussian, as follows:
\[
\hat{b}_i \hat{b}_j^\dagger \hat{\Lambda} = - \partial \hat{\Lambda}. \tag{B38}
\]

**Proof:** The proof can be established easily without Grassmann algebra. We first take the derivative of the unnormalised Gaussian operator:
\[
\partial_{\lambda_{\mu \nu}} \hat{\Lambda} (\sigma) = - \partial_{\lambda_{\mu}} \hat{\Lambda} (\sigma) \hat{b}_\nu. \tag{B39}
\]
We write this as a derivative with respect to the covariance matrix, using Eq. (B41), and swap the pair of operators, to give,
\[
\mathcal{A} \frac{d \hat{\Lambda} (\sigma)}{d \sigma} \mathcal{A} = - \hat{b}_i \hat{b}_j \hat{\Lambda} (\sigma). \tag{B40}
\]
Next, we take the derivative of the normalisation, using Eq. (B39):
\[
\frac{d}{d \sigma} N = \frac{d}{d \sigma} (\pm (\det [i \mathcal{A}])^{-\frac{1}{2}} = - N \mathcal{A}^{-1}. \tag{B41}
\]
Combining both of these results, the derivative of the normalised Gaussian is
\[
\frac{d}{d \sigma} \hat{\Lambda} = -N^{-2} \hat{\Lambda} (\sigma) \frac{dN}{d \sigma} + N^{-1} \frac{d}{d \sigma} \hat{\Lambda} (\sigma)
\]
\[
= \mathcal{A}^{-1} \hat{\Lambda} - \mathcal{A}^{-1} \hat{b}_i \hat{b}_j \mathcal{A}^{-1} \hat{\Lambda}, \tag{B42}
\]
whose inverse is the required result. QED.

This result can also be proved by use of Grassmann coherent-state expansions, in similar manner to the proofs below for the products of different ordering.
6. Mixed products

**Theorem 5:** A product of mixed order of a pair of ladder operators and a Gaussian is equivalent to a first-order differential operator on the Gaussian, as follows:

\[
\left\{ \hat{\beta}_\alpha \hat{\Lambda} : \hat{\beta}^\dagger \hat{\Lambda}_\beta \right\} = -\sigma \Lambda + (\sigma - I) \frac{\partial \Lambda}{\partial \sigma} \sigma. \quad (B43)
\]

**Proof:** We first make use of the Fermi coherent-state completeness identity to replace all ladder operators by Grassmann integrals over coherent projection operators:

\[
\left\{ \hat{\beta}_\alpha \hat{\Lambda} : \hat{\beta}^\dagger \hat{\Lambda} := \int \frac{d\gamma}{d\beta} \frac{d\lambda \alpha d\epsilon}{d\beta} |\gamma\rangle \langle \gamma| \{ \hat{\beta}_\alpha : |\beta\rangle \langle \beta| \hat{\Lambda} \hat{\alpha} : |\alpha\rangle \langle \alpha| \} |\epsilon\rangle \langle \epsilon| \right\}
\]

\[
= \frac{1}{N} \int \frac{d\gamma}{d\beta} \frac{d\alpha \beta d\epsilon}{d\beta} |\gamma\rangle \langle \gamma| \exp \left[ - (\beta, \alpha) (\Lambda + I) \left( \frac{\alpha}{\beta} \right) / 2 \right]
\times \left( \frac{\beta}{\alpha} \right) \left( \beta, \alpha \right) \exp \left[ \gamma \beta + \alpha \epsilon - \alpha \beta - \beta \beta - \frac{1}{2} \gamma \gamma - \frac{1}{2} \epsilon \epsilon \right]
\]

\[
= \frac{1}{N} \left[ \int |\beta \rangle \langle \beta| \hat{\Lambda} \hat{\alpha} : |\alpha\rangle \langle \alpha| \right] |\epsilon\rangle \langle \epsilon| \hat{\Lambda}^{(u)}. \quad (B44)
\]

where we have used the result that the inner product of two coherent states is, from Eq. (A13)

\[
\langle \beta | \alpha \rangle = \exp \left[ \beta \alpha - \beta \beta - \alpha \alpha / 2 \right]. \quad (B45)
\]

Next, we employ integration by parts [Eq. (A1)] to replace \( \left( \frac{\beta}{\alpha} \right) \) by variables that appear in the Gaussian form:

\[
\exp \left[ - (\beta, \alpha) (\Lambda + I) \left( \frac{\alpha}{\beta} \right) / 2 \right]
\times \left( \frac{\beta}{\alpha} \right) \exp \left[ - (\beta \alpha - \beta \beta) \right] (\beta, \alpha)
\]

\[
\exp \left[ - (\beta \beta) \exp \left[ - (\beta \alpha - \beta \beta) \right] (\beta, \alpha)
\]

\[
\exp \left[ \left( \frac{\beta}{\alpha} \right) \exp \left[ - (\beta \alpha - \beta \beta) \right] (\beta, \alpha)
\]

\[
\exp \left[ - (\beta \alpha - \beta \beta) \left\{ \int \frac{d\lambda \alpha d\epsilon}{d\beta} \right\} \left( \beta, \alpha \right) \right]
\times \exp \left[ - (\beta, \alpha) (\Lambda + I) \left( \frac{\alpha}{\beta} \right) / 2 \right]
\]

\[
= \frac{1}{N} \left[ \int |\beta \rangle \langle \beta| \hat{\Lambda} \hat{\alpha} : |\alpha\rangle \langle \alpha| \right] |\epsilon\rangle \langle \epsilon| \hat{\Lambda}^{(u)}. \quad (B44)
\]

where we have used the result that the inner product of two coherent states is, from Eq. (A13)

\[
\langle \beta | \alpha \rangle = \exp \left[ \beta \alpha - \beta \beta - \alpha \alpha / 2 \right]. \quad (B45)
\]

Finally, we can change variables to \( \sigma = |\Lambda + 2I|^{-1} \) and use the result for the derivative of the normalisation:

\[
\left\{ \hat{b}_\alpha : \hat{b}^\dagger \hat{\Lambda}_\beta \right\} = \frac{1}{N} \left[ -(I - \sigma^{-1}) \frac{\partial \Lambda}{\partial \sigma} \sigma - I \hat{\Lambda} \right]
\]

\[
= \frac{1}{N} \left\{ -(I - \sigma^{-1}) \sigma - I \hat{\Lambda} \right\}
\]

\[
= -\sigma \hat{\Lambda} + (\sigma - I) \frac{\partial \Lambda}{\partial \sigma} \sigma. \quad (B48)
\]

QED.

7. Antinormal products

**Theorem 6:** An antinormally ordered product of a pair of ladder operators and a Gaussian is equivalent to a first-order differential operator on the Gaussian, as follows:

\[
\left\{ \hat{b}_\alpha \hat{\Lambda} : \hat{b}^\dagger \hat{\Lambda} \right\} = (\sigma - I) \hat{\Lambda} - (\sigma - I) \frac{\partial \Lambda}{\partial \sigma} \sigma. \quad (B49)
\]

**Proof:** The proof initially proceeds in the same manner as for products of mixed ordering. We first insert the coherent state identity to convert the action of the operators into integrals over coherent-state projectors:

\[
\left\{ \hat{b}_\alpha \hat{\Lambda} : \hat{b}^\dagger \hat{\Lambda} \right\} = \int \frac{d\gamma}{d\beta} \frac{d\alpha \beta d\epsilon}{d\beta} |\gamma\rangle \langle \gamma| \{ \hat{b}_\alpha : |\beta\rangle \langle \beta| \hat{\Lambda} \hat{\alpha} : |\alpha\rangle \langle \alpha| \} |\epsilon\rangle \langle \epsilon|
\]

\[
= \frac{1}{N} \int \frac{d\gamma}{d\beta} \frac{d\alpha \beta d\epsilon}{d\beta} |\gamma\rangle \langle \gamma| \exp \left[ - (\beta, \alpha) (\Lambda + I) \left( \frac{\alpha}{\beta} \right) / 2 \right]
\times \left( \frac{\beta}{\alpha} \right) \exp \left[ \beta \beta - \alpha \alpha - \beta \beta - \frac{1}{2} \gamma \gamma - \frac{1}{2} \epsilon \epsilon \right]
\]

\[
= \frac{1}{N} \left[ \int |\beta \rangle \langle \beta| \hat{\Lambda} \hat{\alpha} : |\alpha\rangle \langle \alpha| \right] |\epsilon\rangle \langle \epsilon| \hat{\Lambda}^{(u)}. \quad (B50)
\]
This time, however, we integrate by parts twice:

\[
\exp \left[ -\left( \beta, \alpha \right) \left( \lambda + I \right) \left( \frac{\alpha}{\beta} \right) / 2 \right] \\
\times \left( \frac{\beta}{\alpha} \right) \left( \lambda, \beta \right) \exp (-\pi \alpha - \beta \alpha)
\]

\[
= \exp \left[ -\left( \beta, \alpha \right) \left( \lambda + I \right) \left( \frac{\alpha}{\beta} \right) / 2 \right] \\
\times \left( -\frac{\partial \beta}{\partial \alpha} \right) \left( \partial \alpha, -\partial \pi \right) \exp (-\pi \alpha - \beta \alpha)
\]

\[
\rightarrow \exp (-\pi \alpha - \beta \alpha) \left( -\frac{\partial \beta}{\partial \alpha} \right) \left( \partial \alpha, -\partial \pi \right)
\]

\[
\times \exp \left[ -\left( \beta, \alpha \right) \left( \lambda + I \right) \left( \frac{\alpha}{\beta} \right) / 2 \right]
\]

\[
= \exp (-\pi \alpha - \beta \alpha) \left[ -\exp \left[ -\left( \beta, \alpha \right) \left( \lambda + I \right) \left( \frac{\alpha}{\beta} \right) / 2 \right] \right]
\]

which is now in a form that we can again express as a derivative of the unnormalised Gaussian operator with respect to \( \lambda \):

\[
\{ \hat{b}^\dagger \hat{b} \lambda \} = -\frac{1}{\mathcal{N}} \int d\gamma d\alpha d\epsilon d\pi |\gamma\rangle \langle \epsilon|
\]

\[
\times \exp \left[ -\pi \alpha - \frac{1}{2} \beta \pi - \gamma \gamma - \frac{1}{2} \pi \epsilon + \gamma \beta + \pi \epsilon \right]
\]

\[
\times \left( \left[ -I + \left( \lambda + I \right) \frac{d}{d\lambda} \right] \exp \left[ -\frac{1}{2} \left( \beta, \alpha \right) \left( \lambda + I \right) \left( \frac{\alpha}{\beta} \right) \right] \right)
\]

\[
\times \left( \lambda + I \right)
\]

\[
= \frac{1}{\mathcal{N}} \left[ -\exp \left( \hat{b}^\dagger \hat{b} \lambda \right) + \left( \lambda + I \right) \frac{d}{d\lambda} \exp \left( \hat{b}^\dagger \hat{b} \lambda \right) \right] \left( \lambda + I \right)
\]

Finally, we change variables to \( \sigma = \left( \lambda + 2I \right)^{-1} \) and use the result for the derivative of the normalisation:

\[
\{ \hat{b}^\dagger \hat{b} \lambda \} = \frac{1}{\mathcal{N}} \left[ -\exp \left( \lambda \hat{\Lambda} \right) + \left( \lambda + I \right) \frac{d}{d\sigma} \exp \left( \lambda \hat{\Lambda} \right) \right] \left( \lambda + I \right)
\]

\[
= \left( \sigma - I \right) \hat{\Lambda} - \left( \sigma - I \right) \frac{d\hat{\Lambda}}{d\sigma} \left( \sigma - I \right).
\]

QED.

(2002).


