Probabilistic Q-function distributions in fermionic phase-space

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Abstract
We obtain a positive probability distribution or Q-function for an arbitrary fermionic many-body system. This is different to previous Q-function proposals, which were either restricted to a subspace of the overall Hilbert space, or used Grassmann methods that do not give probabilities. The fermionic Q-function obtained here is constructed using normally ordered Gaussian operators, which include both non-interacting thermal density matrices and BCS states. We prove that the Q-function exists for any density matrix, is real and positive, and has moments that correspond to Fermi operator moments. It is defined on a finite symmetric phase-space equivalent to the space of real, antisymmetric matrices. This has the natural SO(2M) symmetry expected for Majorana fermion operators. We show that there is a physical interpretation of the Q-function: it is the relative probability for observing a given Gaussian density matrix. The distribution has a uniform probability across the space at infinite temperature, while for pure states it has a maximum value on the phase-space boundary. The advantage of probabilistic representations is that they can be used for computational sampling without a sign problem.

1. Introduction
Phase-space representations of the quantum mechanical density operator were introduced by Wigner [1] and Moyal [2]. Such mappings from quantum mechanics to phase-space have many physical applications, especially in coherence theory [3]. Positive phase-space distributions or Q-functions, introduced by Husimi [4], give mappings which allow quantum mechanical observables to be calculated using probabilistic sampling.

This paper introduces a unique, positive fermionic phase-space representation. This has the same useful properties as other Q-function methods which have been used for bosonic and spin Hilbert spaces. The Q-function derived here is a positive distribution, which is unique once a suitable weight function has been chosen. It is defined for all density matrices, and applicable to fermionic many-body systems. As it is probabilistic, there are no sign problems when sampling the distribution.

Examples of this general approach include the bosonic Q-function [4], the SU(2) Q-function [5, 6], the positive P-function [7], and the general positive distributions over Gaussian operators [8–10]. It is known that the sampling properties of Q-function methods scale favorably in the limit of large systems, which allows high order correlation functions to be computed for large spin systems [11]. Q-functions using atomic coherent states have also been used to study the dynamics of superfluorescence [12–14]. Another application of this type of distribution, based on coherent states for spin and oscillator states, has been used to study quantum dynamics of the Dicke superfluorescence model [15] and thermalization processes [16].

We introduce a general method for constructing such probability distributions, which is not restricted to Fermi systems. Our definition is based on the expectation value of a hermitian operator basis. In the present case, this is the basis of Gaussian fermionic operators [9, 10, 17]. Importantly, we prove that these provide a resolution of unity [18], and have simple differential identities for operator moments. This is fundamental to constructing a useful probabilistic representation.
A Q-function provides a useful method for visualizing and understanding coherence and correlations. It also has potential applications as a computational tool. Since the distribution is always probabilistic, there are no intrinsic sign problems with sampling or Monte Carlo methods. We will treat detailed applications elsewhere.

To achieve this result, we require the representation to satisfy the following three properties, all found with the Husimi function:

1. It exists uniquely for any quantum density-matrix.
2. It is a positive probability distribution.
3. Observables are moments of the distribution.

Can we satisfy these conditions in the case of fermions? Here, we obtain a fermionic Q-function which satisfies the three requirements given above, and show how this fits into a general picture which includes the well-known Husimi function. Our method makes use of a complete set of positive-definite normally ordered operators as a basis [10, 17, 18], and extends the conceptual basis of Q-function methods. The phase-space is a bounded domain of real antisymmetric matrices. We show how the theory of matrix polar coordinates and Riemannian measures on symmetric spaces provides a natural mathematical framework for this probability. Physically, we make use of the class D symmetries introduced by Altland and Zirnbauer [19] to treat normal-superconducting interfaces. We focus on this case, as it is the most general, while bearing in mind that similar results will follow in each of the four symmetry classes of this type.

This paper is organized as follows. In the next section we introduce our general approach of defining a Q-function. In section 3 we describe the general normally ordered Gaussian operators and their properties. In section 4 a completeness proof is given, based on matrix polar coordinate theory. These results are used to define the Q-function in section 5, together with identities for observables and moments. In section 6, we give explicit expressions of the formalism developed here for Gaussian density operators. Section 7 gives a summary of our results and conclusions. Finally, properties of the unitary transformations that we use are proved in appendix A and the inner product of the general Gaussian operators is calculated in appendix B.

2. Generalized Q-function properties

We first introduce a general definition of a positive Q-function representation for any Hilbert space. The approach given here is not just applicable to fermions. It is therefore useful to understand the abstract concepts first. Our approach differs in an essential way from that of Husimi [4] and others [5, 20]. Rather than constructing the phase-space representation using coherent states, we employ a hermitian operator basis. This operator basis can be thought as a basis of coherent operators, rather than coherent states. It is closely related to the more general idea of a Stratonovich–Weyl mapping [21, 22].

2.1. Q-function definition

Suppose we have a positive definite, hermitian operator basis $\hat{A}(\vec{\lambda})$ defined in a Hilbert space $\mathcal{H}$ of quantum mechanical operators, where $\vec{\lambda}$ is a vector in the phase-space domain $D$. We require the following completeness property; the identity operator $\hat{I}$ of the Hilbert space can be resolved as an integral over the phase-space, so that

$$\int_{D} \hat{A}(\vec{\lambda}) d\mu(\vec{\lambda}) = \hat{I}. \quad (2.1)$$

This is called a resolution of unity. Here $d\mu(\vec{\lambda})$ is an associated integration measure on the phase-space. A generalized Q-function is defined as the inner product of the density matrix $\hat{\rho}$ with the operator basis:

$$Q(\vec{\lambda}) = \text{Tr} \left[ \hat{A}(\vec{\lambda}) \hat{\rho} \right]. \quad (2.2)$$

With this definition, condition (1) is automatically satisfied. We will show below that condition (2) is also satisfied. Hence, a Q-function exists for any density matrix in a Hilbert space which has a continuous, positive resolution of the identity operator, proved suitable identities are found that satisfy condition (3).

There is a direct physical interpretation. The operators $\hat{A}(\vec{\lambda})$ are proportional to possible density matrices, and the distribution simply gives the probability density of finding the system in such a state. In the next sections, we demonstrate how the conditions given above can be satisfied in the case of fermions.
2.2. Probability distribution
To demonstrate that the generalized \( Q \)-function defined above has the properties of a probability distribution, as required for condition (2), we must prove that it is positive and normalized for any density matrix.

**Positivity:** since the density matrix \( \hat{\rho} \) is hermitian and positive definite, it must have a diagonal Schmidt decomposition in an orthogonal basis \( \{|n\rangle\} \), as: \( \hat{\rho} = \sum_n \rho_n |n\rangle \langle n| \), where \( \rho_n \geq 0 \). Since \( \hat{A}(\vec{x}) \) is positive definite by assumption, \( \langle n| \hat{A}(\vec{x})|n\rangle \geq 0 \), so that
\[
Q(\vec{x}) = \text{Tr}[\hat{A}(\vec{x}) \hat{\rho}] = \sum_n \rho_n \langle n| \hat{A}(\vec{x})|n\rangle \geq 0.
\]
(2.3)
Thus, the resulting distribution function is positive-semidefinite, as required.

**Normalization:** from the definition given in equation (2.1), it is clear that the trace of any operator can be expressed as an integral over the phase-space, since:
\[
\text{Tr}[\hat{O}] = \int \text{Tr}[\hat{O} \hat{\rho}(\vec{x})] d\mu(\vec{x}). \tag{2.4}
\]
Choosing \( \hat{O} = \hat{\rho} \), it follows that the distribution is normalized to unity, since from equation (2.2):
\[
1 = \text{Tr}[\hat{\rho}] = \int Q(\vec{x}) d\mu(\vec{x}). \tag{2.5}
\]

2.3. Observables and moments
Next, we wish to satisfy condition (3) for the general \( Q \)-function case. This requires the evaluation of observables in the form of \( \text{Tr}[\hat{\rho} \hat{O}_n] = \langle \hat{O}_n \rangle \), and it leads to nontrivial requirements on the basis set. Since the eigenvalue methods used for the Husimi \( Q \)-function are not always available, we look for a more general approach. Proving that these requirements are satisfied in the case of fermions will require an understanding of the differential properties of the fermionic Gaussian operators.

We suppose that there are a complete set of identities that allow all operator moments of physical interest \( \hat{O}_n \) to be mapped into differential operators, so that:
\[
\hat{O}_n \hat{A}(\vec{x}) = D_n(\vartheta_n, \vec{x}) \hat{A}(\vec{x}),
\]
\[
\hat{A}(\vec{x}) \hat{O}_n^+ = D_n^+(\vartheta_n, \vec{x}) \hat{A}(\vec{x}). \tag{2.6}
\]

Here the second equation follows from the first, together with the assumption that the basis set is hermitian. We use the convention that in \( D_n(\vartheta_n, \vec{x}) \), all differential operators are ordered to the left of any functions of \( \vec{x} \). It then follows using the resolution of the identity, equation (2.1), that any observable in the form of an operator moment can be represented as:
\[
\langle \hat{O}_n \rangle = \text{Tr}[\hat{\rho} \hat{O}_n \int \hat{A}(\vec{x}) d\mu(\vec{x})] = \int D_n(\vartheta_n, \vec{x}) Q(\vec{x}) d\mu(\vec{x}). \tag{2.7}
\]
Finally, provided \( D_n(\vartheta_n, \vec{x}) \) can be transformed via integration of the differentials into \( \hat{O}_n(\vec{x}) = D_n(0, \vec{x}) \), with vanishing boundary terms, it follows that:
\[
\langle \hat{O}_n \rangle = \int Q(\vec{x}) \hat{O}_n(\vec{x}) d\mu(\vec{x}) = \langle \hat{O}_n(\vec{x}) \rangle_0 \tag{2.8}
\]
If the differential mappings exist, and the distribution \( Q(\vec{x}) \) allows partial integration, observables can be calculated as a probabilistic distribution of moments over \( \vec{x} \). It is important to choose a phase-space mapping such that \( \hat{O}_n(\vec{x}) \) is efficiently computable.

The set of observables \( \hat{O}_n \) needs to include only the physically relevant moments. If the Hamiltonian has conservation laws, we are usually not interested in their invariant dynamics. This allows one to reduce both the Hilbert space and phase-space dimensionality. Dimension reduction proves useful in the case of the ground state properties of the fermionic Hubbard model, which was numerically solved using fermionic \( P \)-function methods using both translational and number-conservation symmetries [23].

2.4. Bosonic \( Q \)-function
Before examining the fermionic case, we now show that the general definition given above includes the well-known bosonic \( Q \)-function [4] as a special case. In this case the relevant operator basis is a normalized set of bosonic coherent state projectors \(|\vec{a}\rangle \langle \vec{a}|\), which are also used in the Glauber–Sudarshan \( P \)-representation [24, 25]. These are defined in terms of the normalized bosonic coherent states \(|\vec{a}|\), which are eigenstates of the
bosonic annihilation operators, \( \hat{a} = (\hat{a}_1, \ldots, \hat{a}_M) \) with eigenvalues \( \hat{a} = (a_1, \ldots, a_M) \):

\[
\hat{A}_\kappa (\hat{a}) = \frac{1}{\pi^M} |\hat{a}\rangle \langle \hat{a}|.
\] (2.9)

These match our definition: they give a resolution of the identity, since they have the property [24] that

\[
\frac{1}{\pi^M} \int |\hat{a}\rangle \langle \hat{a}| \, d^{2M} \hat{a} = \mathbb{I}.
\] (2.10)

The relevant phase-space of \( \vec{x} \) is the \( M \)-dimensional complex space \( C^M \), and the measure is the standard Euclidean volume measure of \( d^{2M} \hat{a} = \prod_i \, d\alpha_i^{(\text{re})} \, d\alpha_i^{(\text{im})} \) where \( \hat{a} = \alpha_1^{(\text{re})} + i\alpha_1^{(\text{im})} \). From the definition in equation (2.2), one can express the Husimi \( Q \)-function as a unique positive distribution:

\[
Q (\hat{a}) = \frac{1}{\pi^M} \langle \hat{a}| \hat{\rho} |\hat{a}\rangle.
\] (2.11)

In this case, the mappings to observables are also straightforward. For antinormally ordered operators of form \( \hat{O}_{mn} = \prod \hat{a}_i^{m_{ij}} \prod \hat{a}_j^{n_{ij}} \), the corresponding function on phase-space is a c-number moment

\[
O_{mn} (\hat{a}) = \prod \alpha_i^{m_{ij}} \prod \alpha_i^{n_{ij}}, \quad \text{so that}
\]

\[
\text{Tr} \left[ \hat{O}_{mn} \hat{\rho} \right] = \int O_{mn} (\hat{a}) Q (\hat{a}) \, d^{2M} \hat{a}.
\] (2.12)

This result is obtained, as usual, from the application of the eigenvalue equation for the annihilation operators and the definition of the \( Q \)-function.

3. Fermionic Gaussian operators

There have been several previous approaches that have reproduced some, but not all of the properties described in the Introduction. One approach [26] was to directly introduce an \( SU(2) \) based fermion coherent state. This satisfied (1) and (2), but not (3). Subsequently, a \( Q \)-function based on fermionic coherent state projectors was introduced using \( U(N) \) Lie group methods [6, 27–30]. This satisfied (2), but not (1) and (3), since the projectors are not a complete basis, and observables were not derived. A third approach due to Cahill and Glauber [31], used Grassmann coherent states. This approach satisfies (1) and (3) but not (2), as a \( Q \)-function defined this way is Grassmann valued, and therefore neither real nor positive.

Here we define the fermionic \( Q \)-function using the method given above, with fermionic Gaussian operators [17] as a basis. These are also utilized in the complementary fermionic \( P \)-function representations [10], which are non-unique mappings to a phase-space of larger dimension. These have been utilized for evaluating the ground state of the fermionic Hubbard model, via Monte-Carlo techniques [23]. Other applications of these fermionic \( P \)-functions are to the quantum dynamics of Fermi systems, like molecular dissociation [32, 33], and the linear entropy in a quantum phase space [34].

3.1. Quadratic Hamiltonians

Consider a fermionic system composed of \( M \) modes. We define \( \hat{a} \) as a vector of \( M \) annihilation operators and \( \hat{a}^\dagger \) as vector of \( M \) creation operators, where \( \hat{a}_i \) and \( \hat{a}_j^\dagger \) obey the fermionic anticommutation relations:

\[
\{ \hat{a}_i, \hat{a}_j^\dagger \} = \delta_{ij},
\]

\[
\{ \hat{a}_i, \hat{a}_j \} = 0.
\] (3.1)

An extended vector of all \( 2M \) operators is written as \( \vec{\hat{a}} = (\hat{a}_1^\dagger, \hat{a}_2^\dagger, \ldots, \hat{a}_M^\dagger, \hat{a}_M, \ldots, \hat{a}_1) \), while the corresponding adjoint vector is \( \vec{\hat{a}}^\dagger = (\hat{a}_1^\dagger, \hat{a}_2^\dagger, \ldots, \hat{a}_M^\dagger) = (\hat{a}_1^\dagger, \ldots, \hat{a}_M^\dagger, \hat{a}_M, \ldots, \hat{a}_1) \). We denote \( 2M \times 2M \) matrices as \( \hat{H} \), and \( M \times M \) matrices as \( \mathbf{h} \).

The most general quadratic form of the fermion fields, expanded in mode operators, is just the well-known Bogoliubov–de Gennes Hamiltonian:

\[
\hat{H} = \sum_{i,j=1}^{M} \epsilon_i \hat{a}_i^\dagger \hat{a}_j + \frac{1}{2} \left( \Delta_{ij} \hat{a}_i^\dagger \hat{a}_j + \Delta_{ij}^\ast \hat{a}_j^\dagger \hat{a}_i \right).
\] (3.2)

This can written in a compact form as \( \hat{H} = \frac{1}{2} \vec{\hat{a}}^\dagger \hat{H} \vec{\hat{a}} \), where the \( 2M \times 2M \) matrix \( \hat{H} \) is defined as:

\[
\hat{H} = \begin{bmatrix} \mathbf{h} & \mathbf{\Delta} \\ -\mathbf{\Delta}^\ast & -\mathbf{h}^\ast \end{bmatrix}.
\] (3.3)

In order for \( \hat{H} \) to be hermitian, one has the fundamental requirement that \( \mathbf{h} = \mathbf{h}^\ast \). We also require, without loss of generality, that \( \mathbf{\Delta} = -\mathbf{\Delta}^\ast \), since Fermi operators anti-commute. These conditions can be written [19] as
conditions on $H$,

$$H = H^* = -\Sigma H^T \Sigma,$$

(3.4)

where:

$$\Sigma = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \quad (3.5)$$

A Hamiltonian with $\Delta = 0$ is number-conserving, and describes a non-interacting Fermi gas. With $\Delta \neq 0$, this becomes a phase-dependent form appropriate for describing normal-superconductor interfaces, where Cooper pairs can tunnel through a barrier, and is also useful in mean-field treatments of superconductors.

### 3.2. Normally ordered Gaussian operators

Gaussian operators arise in many physical contexts. In analogy with Gaussian distributions in probability theory, these are defined to be exponentials of quadratics in the field operators [9]. Here, we will introduce a unit trace, hermitian Gaussian operator proportional to $\exp (\hat{H})$. Although these also play the role of free-field canonical density matrices, the states that can be represented are completely general.

Our motivation is similar to Glauber’s [24] use of bosonic coherent state projectors, which are also Gaussian operators [8]. Just as with bosons, fermion states with phase-dependent terms do not physically occur in isolated systems. However, they describe coherence properties in the simplest possible way, and provide a complete basis which can be used to represent any density matrix.

It is convenient to parametrize such Gaussian operators as unit-trace normally ordered forms, defined as [10, 17]:

$$\tilde{A} (\sigma) = \sqrt{\det [i \sigma]} \tilde{A}^u (\sigma^{-1} - 2I),$$

(3.6)

where $\tilde{A}^u$ is a normally-ordered but un-normalized Gaussian operator:

$$\tilde{A}^u (\mu) = \exp \left[ -\hat{\sigma}^{\mu} \hat{a}^\dagger \hat{a} / 2 \right],$$

(3.7)

and $I$ is a diagonal matrix given by:

$$I = \begin{bmatrix} -I & 0 \\ 0 & I \end{bmatrix}. \quad (3.8)$$

Here $0$ and $I$ are the $M \times M$ zero and identity matrices, respectively. Normal ordering is denoted by $\ldots$, hence $\hat{a} \hat{a}^\dagger = -\hat{a}^\dagger \hat{a}$, while antinormal ordering is denoted by $\{\ldots\}$, hence $\{\hat{a}^\dagger \hat{a}\} = -\hat{a} \hat{a}^\dagger$.

The $2M \times 2M$ matrix $\sigma = (\mu + 2I)^{-1}$ is the covariance matrix, which has an identical symmetry to $H$. In terms of an $M \times M$ hermitian matrix $n$ and a complex antisymmetric matrix $m$, one can write:

$$\sigma = \begin{bmatrix} n^T - I & m \\ -m^* & I - n \end{bmatrix}. \quad (3.9)$$

In physical terms, the Gaussian operator $\tilde{A}$ is simply the normally ordered density operator of a finite temperature, noninteracting Fermi gas with Hamiltonian proportional to $\tilde{H}$, where $n$ is the normal Green’s function and $m$ the anomalous Greens’ function. These density operators arise in the theory of non-interacting Fermi gases and BCS superconductors.

### 3.3. Differential identities

The normally ordered Gaussian operators have the advantage of having simple differential identities, which will allow us to obtain the $Q$-function observables. These correspond to the action of the extended creation and annihilation operators on the Gaussian basis [10, 17]:

$$\tilde{A} (\sigma) = \sqrt{\det [i \sigma]} \tilde{A}^u (\sigma^{-1} - 2I),$$

(3.6)
Here \( \hat{\sigma} \equiv I - \sigma \). We use nested ordering \([: \ldots :]\) with the convention that external orderings do not change orderings inside internal brackets, and the ordering of \( \hat{A} \) is invariant. When calculating matrix derivatives, we use the convention that:

\[
\frac{\partial}{\partial \sigma_{\mu\nu}} = \delta_{\mu\nu} \delta_{\rho\delta} - \Sigma_{\nu\delta} \Sigma_{\rho\mu}.
\]

(3.10)

### 3.4. Group properties of the Gaussian operators

In order to explain the group properties of the Gaussian operators, we will now consider the non normal ordered Gaussian operator \( \hat{H} \) defined as:

\[
\hat{H} = \exp \left( \hat{a}^\dagger \hat{H} \hat{a} \right).
\]

(3.12)

where \( \hat{H} \) is given by equation (3.3). Following the work of Balian and Brezin [35] on linear transformations of exponentials of quadratic forms, in terms of our notation, we can define the matrix \( T \) as:

\[
T = \exp \left( \hat{H} \right).
\]

(3.13)

This matrix has the following group product law:

\[
T = T^{(1)} T^{(2)}.
\]

(3.14)

The \( T \) matrices therefore form a group equivalent to the special orthogonal \( SO(2M) \) Lie group, since by using a unitary matrix transformation \( U \) we can transform this matrix into a real matrix \( \tilde{T} = U T U^{-1} \) that satisfies \( \tilde{T}^\dagger \tilde{T} = \mathbb{I} \), and \( \det (\tilde{T}) = \exp (\text{Tr} [\hat{H}]) = 1 \). In terms of the Gaussian operators the composition law is:

\[
\hat{R} \left( \hat{H} \right) = \hat{R} \left( \hat{H}^{(1)} \right) \hat{R} \left( \hat{H}^{(2)} \right).
\]

(3.15)

Since the product of two Gaussian operators is also a Gaussian operator, the product is a group operation, and therefore they are another representation of the \( SO(2M) \) Lie group. Hence it also follows that the \( \hat{H} \) matrices are a representation of the \( \mathfrak{so}(2M) \) Lie algebra [36].

The \( \sigma \) and \( \hat{H} \) matrices are related by an isomorphism \( \mathfrak{g} (\hat{H}) = \sigma [37] \), such that the symmetry properties of \( \sigma \) and \( \hat{H} \) are the same. By the arguments given above, \( \sigma \) is another representation of the \( \mathfrak{so}(2M) \) Lie algebra, through its isomorphism with \( \hat{H} \).

The relationship between the two different orderings of the Gaussian operators is [37] \( \mathfrak{g} (\sigma) \hat{A} (\sigma) = \hat{R} (\hat{H}) \), where \( \mathfrak{g} (\sigma) \) is a normalization function. This implies that the normally ordered Gaussian operators are also a representation of the \( SO(2M) \) Lie group. For our purposes, the covariance matrix \( \sigma \) is important, as it will define the Q-function phase-space.

### 3.5. Symmetry classes and transformations

In order to prove our results in later sections, it is useful to relate the Gaussian operators to fundamental results on random matrix ensembles of quantum systems, and the concept of a symmetric space.

Dyson’s ‘threefold way’ [38] classified the possible symmetry groups of random matrix ensembles into real, complex and quaternion types, corresponding to the Weyl classical groups [22]: orthogonal, unitary and symplectic. The physical meaning of these three classes relates to their symmetry properties with respect to behavior under time reversal and spin rotation. Three more ensembles are found when chiral symmetry is included.

The work of Altland and Zirnbauer [19] considered random matrix ensembles in the case of quadratic Hamiltonians for coupled superconductor-normal fermionic systems. These additional, nonstandard symmetry groups are just the transformations of the Gaussian fermionic operators defined above, and give rise
to four new classes of transformations, making ten in all. Each of these Lie groups corresponds to a mathematical symmetric space, which may be considered as a physical phase-space.

The most general of these groups of transformations, which was first analyzed by Balian and Brezin [35], has neither time-reversal nor spin-rotation invariance. This case, known as class D symmetry, allows one to treat an arbitrary Fermi system. All class D type matrices have the symmetry indicated by equation (3.4).

Many physical systems have a higher degree of symmetry. This can be used to reduce the phase-space dimension, which has practical advantages. For example, number conservation and translational symmetry are utilized in Imada’s analysis of the Hubbard model ground state [23], which uses Gaussian operator methods. Such dimension reduction methods can be used for Q-functions also, but we do not treat them here for simplicity.

To obtain expressions which treat particles and holes on an equal basis, we introduce the zeta matrices:

$$\zeta = I - 2a = \bar{a} - a,$$

which we will call ’stretched’ variables. These have an identical class D symmetry.

In order to understand their relationship with the classical symmetry groups, we can transform the Fermi operators to an hermitian Majorana fermion basis, $\tilde{\xi} = U_0 \tilde{d}$. This allows us to introduce a corresponding matrix mapping that preserves quadratic forms:

$$X = i U_0 \zeta U_0^{-1},$$

where the unitary matrix $U_0$ is defined as:

$$U_0 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & i \\ i & -1 \end{bmatrix}.$$  \hfill (3.18)

The class D symmetry properties then become $X = X^* = -XX^T$, which means that $X$ is a $2M \times 2M$ real antisymmetric matrix. These matrices close under commutation and belong to the $so(2M)$ Lie algebra, do the matrices $i\zeta$, which we anticipated in the previous subsection. The same mapping can be used to show explicitly that the $\hat{H}$ matrices are equivalent to real antisymmetric matrices, and hence belong to the $so (2M)$ algebra. While we focus mainly on the usual Fermi operators here, there is an equivalent approach using hermitian Majorana operators and the real antisymmetric $X$ matrices, since this just a unitarily transformed form of $i\zeta$.

An important consequence of this group theoretic correspondence [19] is that there is a unitary matrix $U$ that diagonalizes the matrix $i\zeta$, while retaining the symmetry of equation (3.4). This unitary matrix is a member of the $SO(2M)$ Lie group, with the property that

$$U^{-1}T = U = EUU^T \Sigma.$$  \hfill (3.19)

This requirement means that the unitary transformation $\hat{b} = U \hat{d}$ preserves the Fermi commutators [35].

The preservation of Fermi commutators on the extended vector of operators is essential to the unitary transformations in this paper. It is used in appendix A to show that a normally-ordered Gaussian operator remains normally-ordered in the new variables, after a unitary transformation of both the operators and the covariance matrix.

3.6. Positivity

While $\hat{A}$ is hermitian, is it also positive-definite?

Because not all Gaussian operators $\hat{A}$ of the form given in (3.7) are positive definite, only a finite domain in the phase-space of $\zeta$ variables leads to a physical density matrix with positive eigenvalues. To find a necessary and sufficient restriction, we use the fact that the corresponding covariance $\Sigma$ matrix is hermitian, and so is diagonalizable using the unitary transformation of equation (3.19) to new operators $\hat{b} = U \hat{d}$, leaving the commutation relations invariant.

We show in appendix A that this diagonalizing transformation can be applied inside the normally ordered symbols, and leaves invariant the class D reflection symmetry on the diagonals. After transforming $\zeta$, we obtain

$$U \zeta U^{-1} = \begin{bmatrix} 1 - 2n' \\ 2n' - 1 \end{bmatrix},$$  \hfill (3.20)

where $n'$ is diagonal. On re-ordering the anti-normal terms in the exponential, which requires a sign-change owing to the definition of fermionic normal ordering, the un-normalized Gaussian operator becomes:
\[ \hat{A}^u = \prod_{j=1}^{M} \left[ 1 + \hat{b}_j^* \frac{2n_j - 1}{1 - n_j} \hat{b}_j \right]. \quad (3.21) \]

Noting that the possible eigenvalues of \( \hat{b}_j^* \hat{b}_j \) are 0, 1, we see that the condition \((1 - n') n' > 0\) is both necessary and sufficient for positivity of \( \hat{A}^u \) and hence \( \hat{A} \). Since a unitary transformation does not change the positivity of a matrix, this can be re-written as an equivalent condition on \( \zeta \), defining the phase-space domain \( D \) as:

\[ I_{\zeta} - \zeta^2 > 0. \quad (3.22) \]

The stretched \( \zeta \) matrices therefore have an eigenvalue range from \((-1, 1)\). This domain corresponds to the positive definite hermitian operators of interest. The condition \( I_{\zeta} - \zeta^2 > 0 \) simply means that the matrix \( I_{\zeta} - \zeta^2 \) is positive definite.

### 3.7. Classical domains and symmetric spaces

Since the class D symmetric covariance matrices can be transformed into real antisymmetric \( 2M \times 2M \) matrices using equation (3.17), the hermitian Gaussian operators can also be regarded as having a real phase space of \( M(2M - 1) \) dimensions. The boundary of this space, equivalent to the domain \( D \) of equation (3.22), is defined by the requirement:

\[ \mathcal{R} = I_{\zeta} + \zeta^2 > 0. \quad (3.23) \]

This is the real subspace of the irreducible homogeneous bounded symmetric domain \( R_{III} \) of complex skew-symmetric matrices [39], called a classical domain in the theory of matrix polar coordinates [40]. More generally, all spaces of this type, with Riemannian measure, have a one-to-one relationship with the simple Lie groups that describe physical symmetries. These are called the symmetric spaces [41].

Now the positive-definite nature of \( \mathcal{R} \) means that, amongst other properties, all the diagonal elements are positive. Geometrically, we therefore note the following property in the present case:

\[ \sum_j X_{jj}^2 < 1. \quad (3.24) \]

Thus, every individual element of \( \mathcal{X} \) is bounded, since \( |X_{jj}| < 1 \), and every row and column is bounded by a corresponding hyperspherical shell. This shows that the class D group symmetry properties have a natural correspondence to a phase-space with a finite boundary. There are four similar types of symmetric spaces of this general class, with differing symmetry properties [19]. In principle, any of these can be used to construct a different type of fermionic \( Q \)-function that is appropriate to the relevant symmetry group.

### 4. Resolution of unity

In order to obtain the \( Q \)-function representation, the next step is to obtain a resolution of unity for the normally-ordered fermionic Gaussian operators expressed in terms of the \( \zeta \) matrices. We follow a similar procedure to the parity argument used previously to obtain the resolution of unity for the fermionic Gaussian operators [18]. The main difference is that the present identity requires an integral over a finite domain, due to our choice of a normally ordered basis set.

#### 4.1. Riemannian volume

To carry out integration on the phase-space, it is necessary to obtain a volume measure. Here we follow the original approach of Hurwitz [42, 43] and Hua [40], by using measures defined relative to an invariant metric

\[ ds^2 = \text{Tr} \left( dX^T dX \right) = \text{Tr} \left( d\zeta^* d\zeta \right). \quad (4.1) \]

This gives a unified invariant measure over both the real and complex matrices described above. Given a distance metric, \( ds^2 = g_{ij} dx_i dx_j \), the corresponding Riemannian volume measure is \( d\mu = \sqrt{|g|} \prod dx_i \) [44].
To start with, we define:

\[
\begin{align*}
    \delta X &= \prod_{1 \leq j < k \leq 2M} dX_{jk}, \\
    \delta \zeta &= \prod_{j=1}^{M} d\zeta_j \prod_{1 \leq j < k \leq M} d^2\zeta_{jk} d^2\zeta_{jk+M},
\end{align*}
\]

(4.2)

which are the Euclidean measures for the independent elements of the real anti-symmetric matrix \(X\), and the class D complex matrices respectively.

The volume elements can now be computed. In the antisymmetric case, the metric and corresponding Riemannian measure are

\[
    \delta s^2 = 2 \sum_{1 \leq j < k \leq 2M} dX_{jk}^2,
    \mu(X) = 2^M (M-1/2) \delta X.
\]

(4.3)

For class D hermitian matrices the metric and Riemannian measure are larger, since:

\[
    \delta s^2 = 2 \sum_{j=1}^{M} d^2\zeta_{jj} + 4 \sum_{1 \leq j < k \leq M} \left[ |d\zeta_{jk}|^2 + |d\zeta_{jk+M}|^2 \right],
    \mu(\zeta) = 2^{2M} (M-3/4) \delta\zeta.
\]

(4.4)

Thus, we have now defined the phase-space and a volume measure for the Q-function operator basis.

### 4.2. Matrix polar coordinates

Integration over the phase-space of matrix variables is simplified by using matrix polar coordinates, which are commonly used in random matrix theory \([19, 40, 45]\). Since \(\zeta\) belongs to a Lie algebra, it can be diagonalized, see section (3.5):

\[
    \zeta = U^{-1} \zeta^D U.
\]

(4.5)

Here \(U\) is an element of the \(SO(2M)\) group and \(\zeta^D = \text{diag}(\zeta, -\bar{\zeta})\). The eigenvalues must be in the range \(-1 < \zeta_j < 1\), since the domain is such that \(1 - \zeta_j^2 > 0\). The Jacobian for the transformation from the coordinate \(\zeta\) to polar coordinates \((\zeta, U)\), is given by \([19, 45]\):

\[
    \delta\mu(\zeta) = U^\dagger dU d^2(\zeta^1) d\zeta.
\]

(4.6)

Here we have used the matrix polar coordinate \([19]\) measure for class D symmetry, where \(d\zeta = \prod_{j=1}^{M} d\zeta_j\) and \(\Delta(\zeta^2)\) is the Vandermonde determinant defined as:

\[
    \Delta(\zeta^2) = \prod_{1 \leq i < j \leq M} (\zeta_i^2 - \zeta_j^2) .
\]

(4.7)

To evaluate the Riemannian unitary volume \(C_R = \int (U^\dagger dU)\), we use our previous technique \([18]\) of evaluating a Gaussian integral in both rectangular and polar coordinates over an infinite domain. The integral is:

\[
    G_M = \int_{-\infty}^{\infty} \mu(\zeta) \exp \left[ -\text{Tr} \left( \frac{\zeta \zeta^\dagger}{4} \right) \right] .
\]

(4.8)

From Riemannian volume invariance, this Gaussian integral can be evaluated by unitary transformation to an equivalent real antisymmetric matrix, which gives a one-dimensional real Gaussian integral in each coordinate:

\[
    G_M = \int_{-\infty}^{\infty} \mu(X) \exp \left[ -\text{Tr} \left( \frac{XX^\dagger}{4} \right) / 4 \right] \]

\[
    = 2^M (M-1/2) \int_{-\infty}^{\infty} \exp \left[ -\sum_{i<j}^{2M} \frac{X_{ij}^2}{2} \right] dX
    = (4\pi)^{M(M-1)/2}. \]

(4.9)
Evaluating this using matrix polar coordinates:

\[
G_M = \int \int U^+ dU \int_{-\infty}^{\infty} \Delta^2 (\xi^2) d\xi \exp \left[ -\text{Tr} \left( Y Y' \right) / 4 \right]
\]

\[
= C_R \int_{-\infty}^{\infty} \Delta^2 (\xi^2) d\xi \exp \left[ -\sum_{j=1}^{M} \xi_j^2 / 2 \right].
\] (4.10)

This has the form of a Mehta integral used in random matrix theory [46], and one obtains:

\[
G_M = C_R (2)^{M(M-1)/2} \prod_{j=1}^{M} j! \Gamma (j - 1/2).
\] (4.11)

Hence, on comparing with equation (4.9) we find that the Riemannian unitary volume is given by:

\[
C_R = (2\pi)^{M(M-1)/2} \prod_{j=1}^{M} \frac{1}{j! \Gamma (j - 1/2)}.
\] (4.12)

Since the matrices \( H \) used in [18] also have the class-D symmetry, we can relate this volume to the Euclidean volume \( C_U \) of the class-D matrices derived previously [18]. As expected from equation (4.4), the relation between these two factors is:

\[
C_R = 2^{M(2M-2)} C_U^{1/2}.
\] (4.13)

We can now evaluate the invariant volume \( V = \int_D d\mu (\xi) \) of the classical domain using matrix polar coordinates. In this case we have to evaluate an integral of the form:

\[
V = C_R \int_{-\infty}^{\infty} \Delta^2 (\xi^2) d\xi.
\] (4.14)

In order to perform this integral we consider the following change of variables: \( x_j = \xi_j^2 \), hence \( d\xi_j = \frac{1}{2} x_j^{-1/2} dx_j \). This allows the integral to have the form of a Selberg integral [46]

\[
\int_{-1}^{1} \Delta^2 (\xi^2) d\xi = \int_0^1 \cdots \int_0^1 \left| A (x) \right|^2 \prod_{j=1}^{M} x_j^{-1/2} dx_j.
\]

\[
= \prod_{j=1}^{M} \frac{j! \Gamma (j - 1/2) \Gamma (j)}{\Gamma (M + j - 1/2)}.
\] (4.15)

Using the result of \( C_R \) given in equation (4.12) we obtain that the invariant volume \( V \) of the classical domain is:

\[
V = (2\pi)^{M(M-1)/2} \prod_{j=1}^{M} \frac{(j - 1)!}{\Gamma (M + j - 1/2)}.
\] (4.16)

4.3. Normalized basis

We now wish to prove that a resolution of unity for a suitably normalized Gaussian basis \( \hat{A}^N (\xi) \) is given by:

\[
i = \int_D d\mu (\xi) \hat{A}^N (\xi).
\] (4.17)

The Q-function basis \( \hat{A}^N (\xi) \) that we shall use is a function of the stretched phase-space coordinates \( \xi \) on the classical domain of volume \( V \), which vanishes at the domain boundaries. It is defined as:

\[
\hat{A}^N (\xi) = \frac{1}{\mathcal{N}} \hat{A} \left( \frac{1}{2} \left[ \mathbf{1} - \xi \right] \right) S (\xi^2).
\] (4.18)

Here \( S (\xi^2) \) is an even, positive scaling function, and \( \mathcal{N} \) is a positive constant introduced for normalization purposes.

This basis is positive definite, since the Gaussian operators \( \hat{A} (\xi) \) are positive definite [10, 17], inside the classical domain. The function \( S \) must be invariant under unitary transformations, with a typical general form being:
Using Grassmann variables, it is possible to prove that the normally ordered Gaussian operators can be brought into diagonal form by the unitary transformation of equation (4.5) that diagonalizes the class-D hermitian matrix, and remain normally ordered in the new operator basis. This is shown in appendix A.

The trace normalization term for a Gaussian operator has an equal number of positive and negative eigenvalues. As a result, in terms of the eigenvalues of $\zeta$ and the transformed operators $\hat{b} = U \hat{a} U^{-1}$, the Gaussian operator is:

$$\hat{A} = \det \left[ \frac{1}{2} (I + \xi) \right] \exp \left[ \frac{1}{2} \left( I - (I - \zeta^D)^{-1} \right) \hat{b} \right].$$

(4.20)

In order to obtain the resolution of unity we therefore must prove the following result

$$\hat{I} = \frac{1}{\mathcal{N}} \mathcal{C}_R \hat{\zeta}.$$

(4.21)

Here we have used the matrix polar coordinate Jacobian, equation (4.6), the unitary volume of equation (4.12), and we have introduced a radial integral:

$$\hat{I}_\zeta = \int V \hat{A} (\xi) S (\xi^2) \Delta^2 (\xi^2) d\xi.$$

(4.22)

### 4.4. Radial integral

To complete the proof of the resolution of unity, and obtain the normalizing factor $\mathcal{N}$, we now focus on the radial part. This corresponds to the integral over the eigenvalues $\zeta$. For simplicity in evaluating integrals we will take $\varsigma = 0$ in the normalizing function $S (\xi^2)$. The normally ordered Gaussian operators can be expressed as:

$$\Lambda (\xi) = \exp \left[ 2\hat{b}^\dagger \left( (I + \xi)^{-1} - 1 \right) \hat{b} \right] \det \left[ \frac{1}{2} (I + \xi) \right].$$

(4.23)

Using the result of equations (4.22) and (4.23), we can write the radial integral as:

$$\hat{I}_\zeta = \int V \hat{A} (\xi) S (\xi^2) \Delta^2 (\xi^2) d\xi = 2^{-M} \int_{\xi_j = 0}^1 d\xi^2 (\xi^2) S (\xi^2) \prod_{j=1}^M \zeta_j \left[ \frac{1}{2} - \hat{b}_j \hat{b}_j \right].$$

(4.24)

The value of the integral $\hat{I}_\zeta$ will depend on the normalization function. Expressed in terms of the eigenvalues $\zeta$, this is:

$$S (\xi^2) = \det \left[ (I - \xi^2)^k \right].$$

(4.25)

which is an even function of the eigenvalues.

The second integral of equation (4.24) has terms proportional to $\zeta_j$, which is an odd function of $\zeta_j$, while all the other terms are an even function of $\zeta_j$. Hence from the parity of these functions, the odd integrals vanish, so $\hat{I}_\zeta$ is proportional to a unit operator.

The radial integral which must be evaluated is:

$$I_\zeta = \int_{\xi_j = 0}^1 d\xi^2 (\xi^2) \prod_{j=1}^M \left( 1 - \zeta_j^2 \right)^k.$$

(4.26)

Next we perform the following change of variables: $x_j = \zeta_j^2$, hence $d\zeta_j = \frac{1}{2} x_j^{-1/2} dx_j$. This allows the integral of equation (4.26) to be written in the form:

$$I_\zeta = \int_0^1 \cdots \int_0^1 \mathcal{A}(x)^2 \prod_{j=1}^M x_j^{-1/2} (1 - x_j)^k dx_j,$$
which is another modified Selberg integral \[46\]. Therefore, the radial integral of equation (4.26) is:

\[
I_\gamma = \prod_{j=1}^{M} \frac{j! \Gamma \left( j - \frac{1}{2} \right) \Gamma \left( k + j \right)}{\Gamma \left( k + M + j - \frac{1}{2} \right)},
\] (4.27)

Using the value of \( I_\gamma \) given in equation (4.27), together with the unitary integral, we obtain a general resolution of unity with a normalization constant \( \mathcal{N} \) of the form:

\[
\mathcal{N} = (2\pi)^{M(M-1)/2} 2^{-M} \prod_{j=1}^{M} \frac{\Gamma \left( k + j \right)}{\Gamma \left( k + M + j - \frac{1}{2} \right)}.
\] (4.28)

In the limit of \( k \to 0 \), this normalization constant is just the phase-space volume \( V \) of the real classical domain, divided by the number of many-body quantum states, \( 2^M \). This follows, since the requirement for the resolution of unity, in the limit of \( k, s \to 0 \), is:

\[
\mathcal{N} = 2^{-M} C_R \int_{-1}^{1} d\zeta \zeta \mathcal{A}^2 \left( \zeta^2 \right) = 2^{-M} \int_{V} d\mu (\zeta).
\] (4.29)

The integral on the right hand side is the volume \( V \) of the real classical domain defined in equation (4.16). Hence in the limit of a uniform normalization, we simply have

\[
\lim_{k,s \to 0} \mathcal{N} = 2^{-M} V.
\] (4.30)

A Monte-Carlo integration was carried out to verify this result, by generating \( 10^6 \) random antisymmetric matrices \( \mathcal{X} \) with \(-1 < X_{ij} < 1\), and testing positivity from the eigenvalues. This was in good agreement with equations (4.16) and (4.28) for \( k, M \lesssim 3 \).

These results imply a simple physical interpretation of the resolution of unity. We note that for an arbitrary operator \( \hat{O} \), one immediately obtains from the \( k \to 0 \) limit of the resolution, equation (4.17), that:

\[
\frac{1}{2^M} \text{Tr} \left( \hat{O} \right) = \frac{1}{V} \int_{D} d\mu (\zeta) \text{Tr} \left( \hat{O} \mathcal{A} \left( \frac{\zeta}{2} \right) \right).
\] (4.31)

Hence, the average overlap of any Fermi operator with an orthonormal basis element equals its average overlap with a unit trace Gaussian operator.

5. Fermionic \( Q \)-function and observables

Following the method of section 2, the fermionic \( Q \)-function is now defined inside the volume \( V \) in terms of the normalized Gaussian basis, as:

\[
Q \left( \frac{\zeta}{2} \right) = \text{Tr} \left[ \hat{\rho} \mathcal{A}^N \left( \frac{\zeta}{2} \right) \right].
\] (5.1)

This is the Hilbert–Schmidt inner product of the density operator \( \hat{\rho} \) with the normalized Gaussian basis, \( \mathcal{A}^N = S \hat{\lambda} / \mathcal{N} \), defined in equation (4.18), and hence satisfies our first requirement. The scaling function \( S \) creates a type of gauge symmetry in the representation, since there is a physically equivalent \( Q \)-function representation for every choice of scaling function. Relative to this choice, however, the \( Q \)-function is uniquely determined by the density matrix, as required.

The second requirement was that the \( Q \)-function should be a probability distribution which is normalized to unity. The density matrix \( \hat{\rho} \), is hermitian and positive definite. The general normally ordered Gaussian operators defined in equation (4.18), are hermitian since the matrix \( \zeta \) is hermitian, and they are also positive-definite \([10, 17]\) within the classical domain. Thus, the fermionic \( Q \)-function is a non-negative probability distribution, and it is normalized from the resolution of unity and equation (2.5).

As an example of a \( Q \)-function, the operator \( \hat{I} / 2^M \) is the infinite temperature density matrix with unit trace. This clearly has a constant overlap with any unit trace Gaussian of \( 2^M \). From equation (4.30), in the limit of \( k, s \to 0 \) where \( S = 1 \), one obtains \( Q = 1/V \), as expected for a uniform, normalized probability.

5.1. Differential identities of the fermionic basis

The third required property for a \( Q \)-function is that observables are moments of the distribution. In order to obtain this property, we will use the known differential identities given in equation (3.10), which correspond to the action of the extended creation and annihilation operators on the Gaussian basis \([10, 17]\). In particular, we
will make use of the identity
\[ \{ \hat{a}_i \hat{a}^\dagger_j \} = -\partial_\Lambda^i - \partial_\Sigma_j. \] (5.2)

Here the nested ordering \(|: \ldots :|\) is defined as:
\[ \{ \hat{a}_{ij} \hat{a}^\dagger_{ji} \} = \begin{pmatrix} \hat{a}_i \hat{a}^\dagger_j \Lambda & \hat{a}_i \Lambda \hat{a}^\dagger_j \\ -\hat{a}^\dagger_j \Lambda \hat{a}_i & -\hat{a}^\dagger_j \Lambda \hat{a}_i \end{pmatrix}. \] (5.3)

The derivative of the fermionic Gaussian basis \( \Lambda^N \) with respect to \( \sigma \) is obtained by using the product rule as well as this identity. Hence, the action of the ladder operators on the Gaussian basis \( \Lambda^N \) for this particular nested ordering is given by:
\[ \{ \hat{a}_i \hat{a}^\dagger_j \Lambda^N : \} = -\sigma^{N} - \partial_\Lambda^i - \sigma^{N} \partial_\Sigma_j \sigma^{\Lambda} \ln S. \] (5.4)

5.2. Observables

The extended creation and annihilation operators can be expressed in normal or antinormal form. We will consider the antinormal form of the observables, which are expressed as:
\[ \rho = \frac{1}{2} \{ \hat{a}_i \hat{a}^\dagger_j \}. \] (5.5)

Using the resolution of unity given in equation (4.17) we can write the observables as:
\[ \int \int d\zeta \zeta \rho \hat{a}_i \hat{a}^\dagger_j \Lambda^{N} \zeta = \sigma^{N} \hat{a}_i \hat{a}^\dagger_j \] + \sigma^{N} \partial_\Lambda^i \Lambda^{N} \rho \] + \sigma^{N} \partial_\Sigma_j \sigma^{\Lambda} \ln S. \] (5.6)

Next, substituting the definition of the \( Q \)-function in this expression gives:
\[ \int \int d\zeta \zeta \rho \hat{a}_i \hat{a}^\dagger_j \Lambda^{N} \sigma^{N} \partial_\Lambda^i \Lambda^{N} \sigma^{\Lambda} \ln S. \] (5.7)

On integrating the third term by parts, the boundary term vanishes due to the fact that the scaling factor \( S \) vanishes at the classical domain boundary. Hence for the corresponding bounded classical domain we obtain:
\[ \int d\zeta \zeta \rho \hat{a}_i \hat{a}^\dagger_j \Lambda^{N} \sigma^{N} \partial_\Lambda^i \Lambda^{N} \sigma^{\Lambda} \ln S. \] (5.8)

The results obtained here are independent of the precise form of the weight function \( S \), provided the boundary terms vanish. We now consider the explicit form of the normalization function \( S \), given in equation (4.19), and take the limit of \( k \), \( s \to 0 \) to simplify the result. This limit is taken only after partial integration, so that the
boundary terms vanish as required in our derivation. The matrix derivatives are carried out on making use of equation (3.11), which includes the class-D symmetry property.

Hence, after changing to the stretched variables, the normally ordered Greens functions are given in a simple form by:

\[
\left\{ \hat{a} \hat{a}^\dagger \right\} = C_M \int_{\mathbb{R}^2} \xi Q \left( \frac{\xi}{\mathbb{R}} \right) d\xi - \frac{1}{2} \mathbb{I},
\]

where \( C_M = 2M - 1/2 \) is a constant that depends on the dimensionality. This process can be iterated to obtain higher-order correlations.

In the infinite temperature case of \( Q = 1/\mathbb{V} \), the odd integral on the right-hand side vanishes, which means that \( \langle a_1 a_i \rangle = \langle a_i a_1 \rangle = 1/2 \). This is an expected result due to particle-hole symmetry.

6. Gaussian density operators

In this section we give explicit expressions of fermionic Q-functions in the case of Gaussian density operators. This includes the common cases of a non-interacting thermal gas and a BCS state. More generally, since the Gaussian operators are a complete basis for any density matrix, this allows any Q-function to be calculated if the corresponding fermionic P-function \([10]\) is known. For simplicity, we will consider the limiting normalization with \( k, s \to 0 \), unless stated otherwise.

6.1. Gaussian operator inner product

Consider two normalized Gaussian operators, \( \hat{A} (\xi) \) and \( \hat{A}' (\xi') \). If we consider \( \hat{A} (\xi) \) as the Q-function basis, and \( \hat{A} (\xi') \) as a physical density matrix, then evaluating the Q-function reduces to evaluating their standard Hilbert–Schmidt inner product:

\[
F (\xi, \xi') = \text{Tr} \left( \hat{A} (\xi) \hat{A}' (\xi') \right).
\]

In appendix \( B \), this is carried out following methods previously used to calculate linear entropy \([34]\), together with Grassmann coherent states. This gives the result that:

\[
F = \text{det} \left( \xi - \xi' \right) \left( \mathbb{I} - \xi \right) + \xi' \xi \right)^{1/2},
\]

which takes a simpler form in terms of the stretched variables:

\[
F = 2^{-M} \sqrt{\det \left( \xi + \xi' \xi \right)}.
\]

If the anomalous terms vanish, so that \( m = m' = 0 \), then one obtains:

\[
\xi' \xi \equiv \begin{bmatrix} (I - 2n')^T & (1 - 2n^T) \\ (2n' - I) & (2n - I) \end{bmatrix},
\]

and this reduces to a previously obtained result \([34]\) of:

\[
F = \text{det} \left[ nn^T + (I - n) (I - n') \right].
\]

In the case of a general coordinate \( \xi \), it is instructive to consider the overlap of a density matrix with itself. If we are on the limits of the classical domain, then \( I - \xi^2 = 0 \).

This implies that all the eigenvalues have their extremal values of \( \xi_i = \pm 1 \), which can only occur if there is a unitary transformation that sends every mode into either a ground or excited state, which is a pure state. As a consequence, we expect that \( F = 1 \), since \( F \) is just proportional to the linear entropy. This is exactly the result given by the inner-product expression, equation (6.3).

Thus we see that the classical domain has a clear physical interpretation. It is a domain whose boundary is the Gaussian pure states, with the infinite temperature thermal state of highest entropy at the center.

6.2. Gaussian density operator Q-function

For any Gaussian density operator, like a thermal or BCS state, such that:

\[
\hat{\rho} = \hat{A} (\xi) = \hat{A} \left( \frac{1}{2} \left[ \mathbb{I} - \xi \right] \right),
\]

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the fermionic Q-function in the limit of \( k \to 0 \) has the simple form:

\[
Q \left( \frac{\zeta}{\bar{n}} \right) = \frac{1}{V} \text{det} \left[ \mathbb{I} + \frac{\zeta}{\bar{n}} \right]^{1/2}.
\]  (6.7)

We have already given the simplest example of an infinite temperature state with \( \zeta' = 0 \). The corresponding Q-function is simply the uniform \( Q \)-function, \( Q = 1/V \).

More generally, since any density matrix can be represented [10] using a positive fermionic \( P \)-function \( P ( \zeta ) \) in the stretched coordinates, then any density matrix has a \( Q \)-function given by:

\[
Q \left( \frac{\zeta}{\bar{n}} \right) = \frac{1}{V} \int d \zeta' P \left( \frac{\zeta'}{\bar{n}} \right) \text{det} \left[ \mathbb{I} + \frac{\zeta'}{\bar{n}} \right]^{1/2}.
\]  (6.8)

A special behavior occurs in the case of a pure state, for which \( P ( \zeta ) = \delta ( \zeta - \zeta_p ) \), such that \( \zeta_p = \mathbb{I} \). Let us call the corresponding pure state \( Q \)-function \( Q_p \). Given that it is a pure state \( \zeta_p \), we may wish to evaluate the \( Q \)-function at \( \zeta = \zeta_p \), which physically should be large from overlap arguments. The result can be found using the \( Q \)-function definition of equation (5.1), together with the fact that a pure state density matrix is a projection operator. Alternatively, one can use the Gaussian state result of equation (6.7). Either equation gives the same result: the \( Q \)-function probability is increased by a factor of \( 2^M \) above its value in the highest entropy case:

\[
Q_p \left( \frac{\zeta}{\bar{n}} \right) = \frac{1}{N} = 2^M V.
\]  (6.9)

However, the \( Q \)-function is normalized to unity within the domain \( V \). Therefore, the volume occupied by this high probability peak for a pure state must be relatively small at large \( M \), of order \( 2^{-M} V \).

In the opposite extreme, we can always find an antipodean state. This is exactly on the opposite side of the classical domain boundary, at \( \zeta_a = -\zeta_p \). We note that \( \zeta_a \zeta_p = -\zeta_p^2 = -\mathbb{I} \). Hence, \( Q_p ( \zeta_a ) = 0 \) for this pure state. That is, the \( Q \)-function of a pure state always vanishes at the point antipodean to the original pure state. Physically, this is caused by the fact that in the basis for which the pure state is a number state, the antipodean state has every eigenvalue refl ected, and therefore it is orthogonal.

There are many other orthogonal states to a pure state. In fact, there are \( 2^M - 1 \) orthogonal, pure boundary states \( \zeta_a \) of this type, in which one or more eigenvalues changes sign, leading to a vanishing \( Q \)-function with \( Q_p ( \zeta_a ) = 0 \).

We note that by changing the values of \( k, s \), the detailed shape of the \( Q \)-function can be modified. For example, if \( s \gg 0 \) then the distribution is always concentrated close to the origin, and the high temperature state is a classical Gaussian similar to equation (4.8). If \( s \ll 0 \), the distribution is concentrated at the boundaries, and gives a distribution over pure states.

### 6.3. Single mode Gaussian operators

The normal-ordered single-mode Gaussian operator [17] is a thermal density matrix with fermion number \( n = 1 - \bar{n} \):

\[
\hat{A}_1 (n) = \bar{n}; \quad \exp \left[ -\mathbb{a} \mathbb{a}^\dagger \left( 2 - \frac{1}{\bar{n}} \right) \right] = \left[ \bar{n} + \mathbb{a} \mathbb{a}^\dagger (2n - 1) \right].
\]  (6.10)

Here we consider \( n \) real and \( n \in (0, 1) \); \( n \) gives the number of particles, while \( \bar{n} = 1 - n \) gives the number of holes in the thermal state that corresponds to \( \hat{A}_1 \). As previously, it is useful to define a more symmetric variable, \( \zeta = 1 - 2n \in [-1, 1] \). Following the definition of the fermionic basis given in equation (4.18):

\[
\hat{A}_1^N (\zeta) = \frac{1}{\sqrt{N}} \hat{A}_1 (\zeta) S_1 (\zeta),
\]  (6.11)

where \( S_1 (\zeta) \) is the corresponding normalization function of equation (4.19) for \( M = 1 \). If \( s = 0 \), the normalization function has a particle-hole symmetry, since it is an even function of \( \hat{n} \), given by:

\[
S_1 \left( \zeta \right) = \left( 1 - \zeta \right)^k = 4^k \left( n \bar{n} \right)^k.
\]  (6.12)

For the single mode case the resolution of unity for the phase-space variable \( \zeta \) is given by:

\[
\int_{-1}^1 d\zeta \hat{A}_1^N (\zeta) = \mathbb{I}.
\]  (6.13)

Here we give an explicit proof for resolution of unity for the special case of one mode. Expanding the Gaussian operator, the integral over phase-space is:
\[ \hat{I}_G = \frac{1}{2N} \int_{-1}^{1} \frac{d\zeta}{\tau} \left[ 1 + \zeta - 2\zeta \hat{a}^\dagger \hat{a} \right] S_1 \left( \zeta^2 \right). \]  

(6.14)

The odd-parity integral terms over \( \zeta \) all vanish, including the operator valued part. Hence, to prove a resolution of the identity, it is only necessary to show that:

\[ 1 = \frac{1}{N} \int_{0}^{1} d\zeta \left( 1 - \zeta^2 \right)^k. \]  

(6.15)

A resolution of unity therefore requires a normalization of:

\[ \mathcal{N} = \frac{\sqrt{\pi} k!}{2^{\frac{k}{3}}}. \]  

(6.16)

in agreement with equation (4.28). In the limit of \( k \to 0 \), one has \( \mathcal{N} = \sqrt{\pi}/2 = 1 \).

### Example of thermal states

We will now give an explicit expression for the single-mode Q-function described with this formalism. Since every single mode fermion state is a thermal state, we need only consider the thermal states, with a finite-temperature Fermi–Dirac mean occupation number of:

\[ n_{th} = \frac{1}{\exp \left( (E - \mu)/k_B T \right) + 1}. \]  

(6.17)

The density matrix is itself one of the Gaussian operators:

\[ \hat{\rho}_{th} = \hat{n}_{th} : \exp \left[ -\hat{a}^\dagger \left( 2 - \hat{n}_{th}^{-1} \right) \hat{a} \right] : = \hat{A}_{th} (n_{th} :). \]  

(6.18)

The explicit form of the fermionic Q-function for this case is given by taking the inner product of equation (6.18) and the normalized Gaussian state \( \hat{A}_{th}^N (\zeta) \). The symmetrized thermal occupation is \( \zeta_{th} = 1 - 2n_{th} = 2\tilde{n}_{th} - 1 \). Therefore, in the \( k_s \to 0 \) limit, the Q-function is given by:

\[ Q_{th} (\zeta) = \text{Tr} \left[ \hat{A}_{th} (n_{th}) \hat{A}_{th}^N (\zeta) \right] = \frac{1}{2N} S_1 \left( \zeta^2 \right) \left( 1 + \zeta_{th} \zeta \right). \]  

(6.19)

Here we have used the result for the trace of two normally ordered normalized Gaussian operators [34]. Since \(-1 < \zeta, \zeta_{th} < 1\), the Q function is clearly positive, and the result agrees with the general expression for a multi-mode Gaussian Q-function, equation (6.7).

### Q-function and observables

Using the expression for the observables given in equation (5.2), we can write the corresponding differential identities as:

\[ \hat{a} \hat{a}^\dagger \hat{A}_1 = \left[ \hat{n} - n_{th} \frac{\partial}{\partial n_{th}} \right] \hat{A}_1. \]  

(6.20)

Hence, since the normalization factor is \( \mathcal{N} = 1 \), the observables for the single mode case are:

\[ \langle \hat{a} \hat{a}^\dagger \rangle = \int_{-1}^{1} d\zeta Q (\zeta) \left( \hat{n} + \frac{\partial}{\partial \hat{n}} \left[ \hat{n} + \ln S_1 \right] \right). \]  

(6.21)

On performing the derivatives, taking the limit of \( k \to 0 \) and simplifying terms, we obtain:

\[ \left\{ \hat{a} \hat{a}^\dagger - \frac{1}{2} \right\} = \frac{3}{2} \int_{-1}^{1} \zeta \zeta Q (\zeta) d\zeta. \]  

(6.22)

Using the expression of the Q-function for the thermal state given in equation (6.19) and the expression for the observables given in equation (6.22), we evaluate the observable, which is

\[ \langle 2\hat{a} \hat{a}^\dagger - 1 \rangle_{th} = 3 \int_{-1}^{1} \zeta \zeta Q_{th} (\zeta) d\zeta = \zeta_{th}. \]  

(6.23)

This result corresponds to the expected thermal average value.
7. Summary

In summary, we have introduced a probabilistic fermionic $Q$-function for an arbitrary many body fermionic system. The fermionic $Q$-function is physically interpreted as a suitably normalized overlap of the density operator and the normally ordered Gaussian operators. We have also used three important properties of these Gaussian operators, which are their positivity inside a bounded domain, their resolution of unity and their differential identities. This Gaussian basis is defined with an arbitrary invariant, even weight function, so that they are uniquely defined once this function has been chosen. As a result, we have shown that the $Q$-function is a continuous probability distribution, uniquely defined up to a type of gauge symmetry due to the weight function of the Gaussian basis. It exists for any quantum density matrix and has observables which are moments of the distribution.

The fermionic $Q$-function derived here is a general probabilistic approach to fermion physics. It uses as a complete basis the Gaussian operators, which have been applied in the study of many-body fermionic systems. This is in contrast to previous fermionic $Q$-functions. For example, a $Q$-function defined in terms of anticommuting Grassmann variables is neither a probability nor even a real number.

There is an elegant physical interpretation of the resulting phase-space domain. These Gaussian states are physical states which have the highest possible entropy at the domain centre, and the lowest possible entropy at the boundaries. This is because the classical domain boundary is the set of Gaussian pure states, which includes the BCS states. On the other hand, its centre at $\zeta = 0$ is the infinite temperature thermal state of maximal entropy.

Thus, as a hot fermionic system is cooled, we expect its $Q$-function to be initially uniform on the classical domain, while gravitating towards the boundary as it cools towards states of greater purity.

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Appendix A. Invariance of normal ordering under unitary transformations

In this appendix we prove that any unitary transformation of a class D covariance matrix $\sigma$ that preserves the class D symmetry, leaves the normal ordering form of the Gaussian basis invariant. A similar result to this was obtained by Fan [47]. We note that this result is not generally true for an arbitrary unitary transformation.

In these Appendices, we will use Grassmann algebra methods, and introduce Grassmann coherent states defined as $\alpha \langle \alpha | = \exp [\hat{g}^\dagger \cdot \alpha] | 0\rangle$. Here $\alpha$ is an anti-commuting Grassmann variable with conjugate $\overline{\alpha}$, the eigenvalue equation is $\hat{a} \langle \alpha | = \alpha \langle \alpha |$, and we use the following Grassmann coherent state identities

$$\int d^{2M} \alpha \alpha \alpha \alpha \alpha \alpha \alpha = -I_{A^2},$$

$$\mathcal{M} \mathcal{M} \mathcal{M} \mathcal{M} \mathcal{M} \mathcal{M} \mathcal{M} = -I_{A^2} \mathcal{M} \mathcal{M} \mathcal{M} \mathcal{M} \mathcal{M} \mathcal{M} \mathcal{M}.$$
To prove this result, we will use Grassmann coherent states. The following double Grassmann integral is identical to the Gaussian operator $\Lambda^u$:

$$\hat{I}_A = \int \int d\bar{\alpha} d\beta \langle \alpha | \hat{\Lambda}^u (\mu) | \beta \rangle,$$

where we have introduced the compact notation:

$$\mathcal{Z} = \left( \begin{array}{c} \beta \\ \bar{\alpha} \end{array} \right), \quad d\mathcal{Z} \equiv d^2\alpha d^2\beta.$$

A.2. Gaussian series expansion

We wish to prove that $\hat{I}_A$ and hence $\hat{\Lambda}^u$ is equal to a normally-ordered diagonal Gaussian form. To proceed, $\hat{\Lambda}^u$ inside the integral is expanded as a series of even order normally-ordered polynomials in the Fermi operators, so that:

$$\hat{\Lambda}^u = \sum_{n=0}^{\infty} \frac{2^{-n} p^{(2n)}}{n!}.$$

Using an explicit form of the matrix $\mu$ and recalling that $a = (\hat{a}, \hat{a}^\dagger)$, we can normally order the lowest order quadratic form $P^{(2)}$ of $\hat{\Lambda}^{(u)}$ as:

$$P^{(2)} = \langle \hat{\xi} | \hat{\xi} \rangle \langle \hat{\xi} | \hat{\xi} \rangle^T = \hat{a} \mu \hat{a} + \hat{a}^\dagger \xi \hat{a}^\dagger - \hat{a} \xi \hat{a} + \hat{a} \xi \hat{a}^\dagger.$$

In the last step there is a sign change as well as a transposition, owing to the definition of fermionic normal-ordering, so that $\hat{a} \hat{a}^\dagger = - \hat{a}^\dagger \hat{a}$. From the Grassmann coherent state eigenvalue properties and anticommutation relations, we obtain:

$$- \hat{a} \xi \hat{a}^\dagger | \beta \rangle = - \beta^T \xi^T | \beta \rangle$$

$$\langle \alpha | \hat{a}^\dagger \xi \hat{a} \rangle = \langle \alpha | \mu \xi \rangle,$$

and applying this to all terms:

$$\langle \alpha | \hat{\Lambda}^u | \beta \rangle = \langle \alpha | \xi \rangle \mathcal{Z}^T \mathcal{Z} \sum \mathcal{Z}^T \mathcal{Z},$$

where $\sum$ is the transposition matrix defined in the main text.

For higher order polynomials, an analogous procedure occurs. There will be an even number of sign changes for both Fermi operator re-orderings and for Grassmann variable re-orderings. Hence:

$$\langle \alpha | \hat{\Lambda}^u | \beta \rangle = \exp \left[ - \frac{1}{2} \xi^T \sum \xi \right] \langle \alpha | \beta \rangle.$$

A.3. Unitary transformations

So far we have expressed the un-normalized Gaussian operator term in terms of Grassmann variables. Next, we are going to consider the class-D unitary transformations that diagonalize the matrix $\mu$ under consideration. This is a $2M \times 2M$ unitary transformation of the Fermi operators:

$$\left( \begin{array}{c} \hat{b} \\ \hat{b}^\dagger \end{array} \right) = U \left( \begin{array}{c} \hat{a} \\ \hat{a}^\dagger \end{array} \right).$$

Note that if we diagonalize the matrix $\mu$ we also diagonalize the matrix $\sigma$. As pointed out by Altland and Zirnbauer [19], $U$ must satisfy $U = \Sigma U^T \Sigma$ with:

$$U = \begin{bmatrix} u^{11} & u^{12} \\ u^{21} & u^{22} \end{bmatrix}.$$

This property implies that:

$$\begin{bmatrix} u^{11} & u^{12} \\ u^{21} & u^{22} \end{bmatrix} = \begin{bmatrix} u^{22} & u^{11} \\ u^{12} & u^{21} \end{bmatrix}.$$
which guarantees that the transformation, when applied to the Fermi operators, preserves operator commutators [35]. We can apply the same transformation to the Grassmann variables, by choosing that

\[ \begin{pmatrix} \beta' \\ \alpha' \end{pmatrix} = U \begin{pmatrix} \beta \\ \alpha \end{pmatrix}, \]

\[ \begin{pmatrix} \alpha' \\ \beta' \end{pmatrix} = U \begin{pmatrix} \alpha \\ \beta \end{pmatrix}. \]  

(A.15)

From the first expression, one obtains:

\[ \alpha' = u^{12}\beta + u^{21}\alpha, \]  

(A.16)

while on conjugating the second expression:

\[ \alpha'^* = u^{12}\beta + u^{21}\alpha = u^{21}\beta + u^{12}\alpha = \alpha'. \]  

(A.17)

This means that the transformation is a consistent transformation on Grassmann variables that preserves conjugation, so that if \(|\alpha'\rangle\) is the new coherent state in the new basis, then:

\[ |\alpha\rangle = |\alpha'\rangle. \]  

(A.18)

Therefore, the Grassmann quadratic in the exponential is also diagonalized by the unitary transformation, so that:

\[ \gamma^T \Sigma \gamma = \gamma'^T \Sigma \gamma' = -2\alpha \lambda \beta'. \]  

(A.19)

It follows that one can extend this argument to each even order polynomial form in the exponential, so that:

\[ \exp \left[ -\frac{\gamma^T \Sigma \gamma}{2} \right] = \exp \left[ -\frac{\gamma'^T \Sigma \gamma'}{2} \right]. \]  

(A.20)

A.4. Gaussian in operator form

We can now evaluate the Grassmann integral, noting that the integration measure is invariant under a unitary transformation, since it has unit Jacobian:

\[ \int \int |\alpha| \langle \alpha | \exp \left[ -\frac{\gamma^T \Sigma \gamma}{2} \right] |\beta \rangle \langle \beta | = \int \int |\alpha'\rangle \langle \alpha' | \exp \left[ -\frac{\gamma'^T \Sigma \gamma'}{2} \right] |\beta' \rangle \langle \beta' |. \]  

(A.21)

We can now use the eigenvalue properties of the Grassmann coherent states in the transformed basis to return back to the operator form in the diagonal basis, so that, on making use of the Grassmann coherent state expansion of the identity, one obtains:

\[ \hat{\Lambda}^{(u)} = \int \int |\alpha'\rangle \langle \alpha' | \cdot \exp \left[ -\frac{\hat{b}^T \Sigma \hat{b}}{2} \right] |\beta' \rangle \langle \beta' | = \cdot \exp \left[ -\frac{\hat{b}^T \Sigma \hat{b}}{2} \right]. \]  

(A.22)

This means that we have the required result. That is, we can diagonalize the class-D covariance matrix for the normally-ordered Gaussian operators using the same transformations used in [18], while leaving the underlying normally-ordered form invariant, just as one can in a non-normally-ordered case.

Appendix B. Inner product of two Gaussian operators

Consider two normalized Gaussian operators, \( \hat{\Lambda}(\sigma) \) and \( \hat{\Lambda}(\sigma') \). We wish to evaluate their standard Hilbert–Schmidt inner product:

\[ F(\sigma, \sigma') = \text{Tr} \left( \hat{\Lambda}(\sigma) \hat{\Lambda}(\sigma') \right). \]  

(B.1)

We will start by evaluating the inner product of the two corresponding un-normalized operators, \( \hat{\Lambda}^{\mu}(\mu) \) and \( \hat{\Lambda}^{\mu'}(\mu') \), where:

\[ F^\mu(\mu, \mu') \equiv \text{Tr} \left( \hat{\Lambda}^{\mu}(\mu) \hat{\Lambda}^{\mu'}(\mu') \right). \]  

(B.2)

We now use the known result for a trace, and the expansion of the identity operator in Grassmann variables, so that:
\[ F^{\alpha} (\mu, \mu') = \int d^{2M} \alpha \langle -\alpha | \hat{A}^{\alpha} (\mu) \hat{A}^{\alpha} (\mu') | \alpha \rangle \]
\[ = \int d^{2M} \alpha d^{2M} \beta \langle -\alpha | \hat{A}^{\alpha} (\mu) | \beta \rangle \langle \beta | \hat{A}^{\alpha} (\mu') | \alpha \rangle. \quad (B.3) \]

From the inner product properties of the Grassmann coherent states
\[ \langle \beta | \alpha \rangle = e^{\frac{i}{2} [\beta, \alpha]} \]
\[ = e^{\frac{i}{2} [\beta, \alpha]} \quad (B.4) \]

Now, on taking account of normal ordering, together with the eigenvalue properties of the coherent states, one can write that:
\[ \langle \beta | \hat{A}^{\alpha} (\mu) | \alpha \rangle = \langle \beta | \alpha \rangle \exp \left[ -\frac{\beta, \alpha}{2} \right] \]
\[ = e^{-\frac{1}{2} [\beta, \alpha]} \quad (B.5) \]

Similarly, for the other term
\[ \langle -\alpha | \hat{A}^{\alpha} (\mu) | \beta \rangle = \langle -\alpha | \beta \rangle \exp \left[ -\frac{\alpha, \beta}{2} \right] \]
\[ = e^{-\frac{1}{2} [\alpha, \beta]} \quad (B.6) \]

**B.1. Sign reversal variable change**

It is convenient at this stage to make a variable change of \( \alpha = -\alpha' \), noting that in Grassmann calculus, the conjugate variable can be regarded as an independent complex variable. This causes a sign change in the integration of \((-1)^M\). As a result, we can introduce a new variable
\[ \mathcal{Z} = \begin{pmatrix} \alpha \\ \hat{\beta} \\ \beta \\ \alpha' \end{pmatrix}, \quad (B.7) \]
and its conjugate, which is:
\[ \mathcal{Z}^\dagger = [\alpha', \beta, \hat{\beta}, \alpha]. \quad (B.8) \]

We note that \( d^{2M} \alpha d^{2M} \beta = (-1)^M d^{2M} \alpha d^{2M} \hat{\beta} = d^{4M} \mathcal{Z} \), since the sign change and the Grassmann reordering in the integration variables will cancel each other. As a result, we can write that
\[ F^{\alpha} (\mu, \mu') = \int d^{4M} \mathcal{Z} \exp \left[ -\frac{1}{2} \mathcal{Z} \Gamma \mathcal{Z}^\dagger \right], \quad (B.9) \]
where \( \Gamma \) is a \( 4M \times 4M \) matrix, such that:
\[ \Gamma = \begin{pmatrix} I & I + \mu \\ I + \mu' & -I \end{pmatrix}. \quad (B.10) \]

**B.2. Grassmann integration result**

This is a standard Grassmann Gaussian integral, except that it is in a space of twice the previous dimension. Hence, the inner product is a Pfaffian of the antisymmetrized form of \( \Gamma \), given as a determinant by:
\[ F^{\alpha} = \det \left[ (I + \mu')(I + \mu) + \frac{1}{2} \Gamma \right]^{1/2}. \quad (B.11) \]

Now, changing variables to the covariance matrix, one obtains:
\[ \mathcal{I} + \mu = \mathcal{I}^{-1} - \mathcal{I}, \quad (B.12) \]
so that in terms of these variables
\[ F^{\alpha} = \det \left[ (\mathcal{I}^{-1} - \mathcal{I})(\mathcal{I}^{-1} - \mathcal{I}) + \frac{1}{2} \right]^{1/2}. \]
Hence, multiplying by the normalizing factors of $\sqrt{\det[i\sigma_2]}$, and noting that $(-1)^{2M} = 1$, one obtains:

$$F = \det\left[\left(\mathbb{I} - \frac{a'}{a}\right)\left(\mathbb{I} - \frac{a}{a'}\right) + \frac{a}{a'}\frac{a'}{a}\right]^{1/2}. \quad (B.13)$$

This can also be written in terms of the stretched variables, $\zeta = \mathbb{I} - 2a$. We note that:

$$\left(\mathbb{I} - \frac{a'}{a}\right)\left(\mathbb{I} - \frac{a}{a'}\right) = \frac{1}{4}\left(\mathbb{I} + \zeta\right)\left(\mathbb{I} + \zeta'\right)$$

$$\frac{a}{a'}\frac{a'}{a} = \frac{1}{4}\left(\mathbb{I} - \zeta\right)\left(\mathbb{I} - \zeta'\right)$$

to give the result that:

$$F = 2^{-M}\sqrt{\det\left[\mathbb{I} + \zeta + \zeta'\right].} \quad (B.14)$$

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