Quantum fidelity for arbitrary Gaussian states

Leonardo Banchi,1 Samuel L. Braunstein,2,3 and Stefano Pirandola2,3

1Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT
2Department of Computer Science, University of York, York YO10 5GH, United Kingdom
3York Centre for Quantum Technologies (YCQT), University of York, York YO10 5GH, United Kingdom

We derive a computable analytical formula for the quantum fidelity between two arbitrary multimode Gaussian states which is simply expressed in terms of their first- and second-order statistical moments. We also show how such a formula can be written in terms of symplectic invariants and used to derive closed forms for a variety of basic quantities and tools, such as the Bures metric, the quantum Fisher information and various fidelity-based bounds. Our result can be used to extend the study of continuous-variable protocols, such as quantum teleportation and cloning, beyond the current one-mode or two-mode analyses, and paves the way to solve general problems in quantum metrology and quantum hypothesis testing with arbitrary multimode Gaussian resources.

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I. INTRODUCTION

The quantification of the similarity between two quantum states is a crucial issue in quantum information theory [1,2] and, more generally, in the entire field of quantum physics [3]. Among the various notions, that of quantum fidelity [4,5] is perhaps the most well-known for its use as a quantifier of performance in a variety of quantum protocols. Quantum fidelity is the standard tool for assessing the success of quantum teleportation [6,7], where an unknown state is destroyed in one location and reconstructed in another (see Ref. [12] for a recent review). In quantum cloning [13–17], where an unknown state is transformed into two or more (imperfect) clones, quantum fidelity is the basic tool to quantify the performance of a quantum cloning machine. Quantum fidelity plays a central role in quantum metrology [18,19], where the goal is to find the optimal strategy to estimate a classical parameter encoded in a quantum state. Similarly, it is important in quantum hypothesis testing [20,21], where the aim is to optimize the discrimination of quantum hypotheses (states or channels).

An important setting for all the above tasks is that of continuous-variable systems [22,23], which are quantum systems with infinite-dimensional Hilbert spaces, such as the bosonic modes of the electromagnetic field, described by position and momentum quadrature operators. For these systems, Gaussian states [22] are the most typical quantum states in theoretical studies and experimental implementations, so quantifying their similarity is of paramount importance. The derivation of a simple formula for the quantum fidelity between two arbitrary bosonic Gaussian states is a long-standing open problem with a number of partial solutions accumulated over the years. We currently know the solutions for one mode [25–27] and two modes [28]. A simple formula for multimode Gaussian states is only known in specific cases, namely when one of the two states is pure [29] or for two thermal states [30].

Here we solve this long-standing problem by deriving a computable formula for the quantum fidelity between two arbitrary multimode Gaussian states which is simply expressed in terms of their first- and second-order statistical moments. A key step for this derivation relies on the adoption of an exponential Gibbs-like representation for the Gaussian states, which has been used recently to evaluate the fidelity between fermionic Gaussian states [24], and which allows us to simplify many calculations. We also provide a recipe for expressing the quantum fidelity in terms of symplectic invariants, showing specific examples with one, two and three modes. The new formula for the fidelity allows us to easily derive the Bures metric for Gaussian states, therefore generalizing quantum metrology to multimode Gaussian resources. Similarly, we discuss how quantum hypothesis testing can be extended beyond two-mode Gaussian states.

II. PRELIMINARY NOTIONS

Consider n bosonic modes described by quadrature operators \( Q = (x_1, \ldots, x_n, p_1, \ldots, p_n)^T \), satisfying the canonical commutation relations [31]

\[
[Q_l, Q^T_k] = i\Omega_{lk}, \quad \Omega := \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \otimes I,
\]

where \( I \) is the \( n \times n \) identity matrix. The coordinate transformations \( Q' = S Q \) which preserve the above commutation relations form the symplectic group, i.e. the group of real matrices such that \( S \Omega S^T = \Omega \) [32].

Let us denote by \( \hat{\rho} \) an unnormalized density operator of the \( n \) bosonic modes. Its normalized version is denoted by \( \rho = \hat{\rho} / Z_\rho \), with \( Z_\rho = \text{Tr} \hat{\rho} \) being the normalization factor. For a Gaussian state [22], the density operator \( \hat{\rho} \) has a one-to-one correspondence with the first- and second-order statistical moments of the state. These are the mean value \( \mu := (Q)_\rho \in \mathbb{R}^{2n} \) and the covariance matrix (CM) \( V \), with generic element

\[
V_{kl} = \frac{1}{2} \langle [Q_k - u_k, Q_l - u_l]_{\rho} \rangle,
\]

where \( \{,\} \) is the anticommutator. Equivalently, we may use the following modified version of the CM

\[
W := -2Vi\Omega.
\]
According to Williamson’s theorem, there exists a symplectic matrix $S$ such that \[ V = S(D \oplus D)S^T, \quad D = \text{diag}(v_1, \ldots, v_n), \] (4) where the symplectic eigenvalues satisfy $v_k \geq 1/2$. Correspondingly, the matrix $W$ transforms as $SWS^{-1}$ and its standard eigenvalues are $\pm w_k$ where $w_k = 2v_k \geq 1$.

In Appendix A, we show that an arbitrary multimode Gaussian state with mean $\mu$ and CM $V$ can be written in the exponential form \[ \rho = \exp \left[ -\frac{1}{2}(Q - \mu)^T G(Q - \mu) \right], \quad Z_{\rho} = \det \left( V + i\Omega/2 \right)^{1/2}, \] (5) where the Gibbs matrix $G$ is related to the CM by the formulae \[ G = 2i\Omega \coth^{-1}(2V\Omega), \quad V = \frac{1}{2} \coth \left( \frac{4G}{2} \right) \Omega. \] (6) Equivalently, we may consider the following relations \[ e^{i\Omega G} = W - \mathbb{I} \frac{W + \mathbb{I}}{2}, \quad W = \mathbb{I} + e^{i\Omega G} \mathbb{I}, \] (7) \[ -\frac{1}{2}(Q - \mu^T G(Q - \mu)) \]

we use the notation $A/B := AB^{-1}$ when $A$ and $B$ commute – see Appendix B for more details. Although the matrix $G$ is singular for pure states (so one has to deal carefully with this limit), the introduction of the representation in Eq. (5) significantly simplifies the calculations, and all the final formulae are valid in general, i.e., for both mixed and pure states.

### III. FIDELITY FOR MULTIMODE GAUSSIAN STATES

The quantum fidelity between two arbitrary quantum states, $\rho_1 = \rho_1/Z_{\rho_1}$ and $\rho_2 = \rho_2/Z_{\rho_2}$, is given by \[ F_0(\rho_1, \rho_2) := \text{Tr} \left( \sqrt{\sqrt{\rho_1} \rho_2 \sqrt{\rho_1}} \right) = \frac{Z_{\rho_1} \rho_{\text{tot}}}{\sqrt{Z_{\rho_1} Z_{\rho_2}}}, \] (8) where $\rho_{\text{tot}} := \sqrt{\rho_1 \rho_2} \sqrt{\rho_1}$. We consider two Gaussian states, $\rho_1$ with CM $V_1$ and mean $\mu_1$, and $\rho_2$ with CM $V_2$ and mean $\mu_2$. The Gibbs matrices $G_1$ and $G_2$ are readily obtained from Eqs. (6) and (7). The advantage of the Gibbs representations (5) for the calculation of the fidelity is twofold: firstly, it makes the evaluation of the operator square root in Eq. (8) straightforward, and secondly, one can use the algebra of quadratic operators [33] to find $\rho_{\text{tot}}$ in a closed form. As we show in Appendix C, given two generally-displaced Gaussian states, the formula for their quantum fidelity can be directly expressed in terms of $\delta_u := u_2 - u_1$ and their CMs, $V_1$ and $V_2$. In fact, we find \[ F_0(\rho_1, \rho_2) = F_0(V_1, V_2) \exp \left[ -\frac{1}{4} \delta_u^T (V_1 + V_2)^{-1} \delta_u \right], \] (9) where the term $F_0(V_1, V_2)$ depends only on $V_1$ and $V_2$ and is easily computable from one of the two auxiliary matrices \[ V_{\text{aux}} = \Omega^T (V_1 + V_2)^{-1} \left( \frac{\Omega}{4} + V_2 \Omega V_1 \right), \] (10) \[ W_{\text{aux}} := -2V_{\text{aux}} \Omega = -(W_1 + W_2)^{-1} (W_1 + W_2 W_1). \] (11) More precisely, we find \[ F_0(V_1, V_2) = \frac{F_{\text{tot}}}{\sqrt{\det (V_1 + V_2)}}, \] (12) \[ F_{\text{tot}} = \det \left[ 2 \left( \sqrt{\frac{1}{2} (\frac{V_{\text{aux}} \Omega}{4} + 1) V_{\text{aux}}} \right)^2 - 1 \right] \] (13) \[ F_{\text{tot}} = \det \left( \sqrt{\frac{1}{2} (W_{\text{aux}} - W_{\text{aux}}^T) V_{\text{aux}} + 1} \right) W_{\text{aux}} \Omega. \] (14)

Note that the asymmetry of $V_{\text{aux}}$ and $W_{\text{aux}}$ upon exchanging the two states is only apparent and comes from the apparent asymmetry in the definition of Eq. (8). One can check that the eigenvalues of $V_{\text{aux}}$ and $W_{\text{aux}}$, and thus the determinants in Eqs. (13) and (14), are invariant under exchange. We remark that the formula of Eq. (9) is valid for arbitrary (generally-displaced) multimode Gaussian states with arbitrary first- and second-order moments. In the specific case where one of the states is pure (say $\rho_1$), we have $V_1 = \mathbb{I}/2$ which implies $V_{\text{aux}} = \mathbb{I}/2$ and $F_{\text{tot}} = 1$, therefore recovering the recent result of Ref. [29] (in different notation [34]).

### IV. FIDELITY IN TERMS OF SYMPLECTIC INVARIANTS

The fidelity can be expressed in terms of symplectic invariants associated with the second-order moments of the Gaussian states. Consider the notation with the W-matrices, so that $F_{\text{tot}}$ is given by Eq. (11). The standard eigenvalues of $W_{\text{aux}}$ are $\pm w_k$, where $w_k \geq 1$ [35]. As a consequence, we may write \[ F_{\text{tot}} = \prod_{k=1}^n w_k^{2} + \sqrt{(w_k)^2 - 1}^{1/2}. \] (15)

Thus, the problem reduces to finding the eigenvalues of $W_{\text{aux}}$. For this, let us consider the characteristic polynomial \[ \chi(\lambda) = \det (\lambda \mathbb{I} - W_{\text{aux}}), \] (16) which is clearly a symplectic invariant since $W_{\text{aux}}$ transforms as $SW_{\text{aux}}S^{-1}$ under symplectic transformations. Using the identity $\det e^{X} = e^{\text{tr}X}$ and the Cayley-Hamilton theorem [36], we may write $\chi(\lambda)$ as a polynomial function of \[ I_{2k} = \text{Tr}(W_{\text{aux}}^{2k}), \quad k = 1, \ldots, n, \] (17) which are also symplectic invariants with $I_k > I_j$ for $k > j$. Thus, for $n$ modes, we can compute the $n$ invariants $I_{2k}$ and subsequently solve the polynomial equation $\chi(\lambda) = 0$, whose roots are the eigenvalues $w_k$ to be used in Eq. (15). Note that the invariants $I_{2k}$ can be connected with other invariants. For instance, one can easily check that $\chi(0) = (-1)^n \Delta$, $\chi(1) = (-1)^n \frac{\Lambda}{\Delta}$, (18) where $\Delta := \det (V_1 + V_2)$, $\Lambda := 2^n \det (\Omega V_1 \Omega V_2 - \mathbb{I}/4)$ and $\Lambda := 2^n \det (V_1 + i\Omega/2) \det (V_2 + i\Omega/2)$, (19) are the invariants considered by Ref. [28]. Using Eq. (18), one can easily express $I_2$ and $I_4$ in terms of $\Gamma$, $\Lambda$ and $\Delta$. 

\[ \text{(19)} \] \[ \text{(20)} \] 

\[ \text{(21)} \]
V. EXAMPLES

Let us show some examples with \( n = 1, 2 \) and 3 modes. For single-mode Gaussian states, we derive \( \chi(\lambda) = \lambda^2 - I_2/2 \), so that \( w_{\text{aux}}^\pm = \sqrt{I_2/2} \). Equivalently, we may compute \( I_2/2 = 1 + \lambda/\lambda \) so that we retrieve the known result \([23, 27]\)

\[
\mathcal{F}_0^2(V_1, V_2) = \frac{1}{\sqrt{\lambda + \lambda - \sqrt{\lambda}}}.
\]

(20)

For two-mode Gaussian states, we derive \( \chi(\lambda) = (I_2^2 - 2I_4 - 4I_2\lambda^2 + 8\lambda^4)/8 \) with solutions

\[
w_{\text{aux}}^\pm = \pm \frac{1}{2} \sqrt{I_2 \pm \sqrt{4I_4 - I_2^2}}.
\]

(21)

Once plugged into Eq. (15), we have the fidelity in terms of \( \Gamma/\lambda \) and \( \lambda/\lambda \), the latter invariants can then be expressed in terms of \( \Gamma/\lambda \) and \( \lambda/\lambda \), so that we retrieve the known result \([28]\)

\[
\mathcal{F}_0^2(V_1, V_2) = \frac{1}{\sqrt{\lambda + \lambda - \sqrt{(\lambda + \lambda)^2 - \lambda}}}.
\]

(22)

For three-mode Gaussian states, the characteristic polynomial may be written as \( \chi = \lambda^3 + pt + q \), where

\[
t = \lambda^2 - I_2/6, \quad p = \frac{I_2^2}{24} - \frac{I_4}{4}, \quad q = -\frac{I_2^2}{108} + \frac{I_2I_4}{12} - \frac{I_6}{6}.
\]

(23)

The solutions of the characteristic equation \( \chi = 0 \) are real (see Appendix D) and given by

\[
w_{\text{aux}}^k = \pm \frac{1}{2} \sqrt{I_2 \pm \sqrt{-p/3 \cos \left( \frac{\theta - 2\pi(k - 1)}{3} \right)}}.
\]

(24)

where \( \theta := \arccos \left[ \frac{3}{\sqrt{3}} q(2p - \sqrt{p})^{-1} \right] \) and \( k = 1, 2, 3 \) (in particular, note that \( w_{\text{aux}}^k = \sqrt{I_2/6} \) for \( p = 0 \)). To the best of our knowledge, Eqs. (23) and (24), together with Eqs. (9) and (15), provide the first expression for the quantum fidelity between two arbitrary three-mode Gaussian states.

VI. IMMEDIATE IMPLICATIONS

A. Geometry of Gaussian states

Once the quantum fidelity is expressed in terms of the first two statistical moments, we can easily compute the Bures distance between two arbitrary multimode Gaussian states, \( \hat{\rho}_1 \) and \( \hat{\rho}_2 \), which is given by

\[
D_B(\hat{\rho}_1, \hat{\rho}_2) = 2 \left[ 1 - \mathcal{F}(\hat{\rho}_1, \hat{\rho}_2) \right].
\]

(25)

Form this expression we can derive the Bures metric by expanding the fidelity. In fact, let us consider two infinitesimally-close Gaussian states \( \hat{\rho}_1 = \hat{\rho} + d\hat{\rho} \), with statistical moments \( u + du \) and \( V + dV \). Then, the Bures metric is given by

\[
ds^2 = 2\left[ 1 - \mathcal{F}(\hat{\rho} + d\hat{\rho}, \hat{\rho} + d\hat{\rho}) \right] = \frac{duV^{-1}du}{4} + \frac{\delta}{8},
\]

(26)

where \( \delta := 4 \text{Tr}[dV(4\mathcal{L}_X + \mathcal{L}_\lambda)^{-1}dV] \). \( \mathcal{L}_X := AXA \), and the inverse of the superoperator \( 4\mathcal{L}_X + \mathcal{L}_\lambda \) refers to the pseudo-inverse \([30]\) (see Appendix E for the proof). Note that a result equivalent to Eq. (26) has been derived in Ref. \([37]\) using a different method based on the computation of the symmetric logarithmic derivative.

Numerically, the easiest way of evaluating the inverse of the superoperator in \( \delta \) is using the \( W \)-matrices and performing the calculations in the basis in which \( W \) is diagonal. In the basis where \( W \) is diagonal, then

\[
\delta = \sum_{i,j} dW_{ij}dW_{ij}^{-1},
\]

(27)

and the sum is taken over the elements such that \( w_iw_j \neq 1 \). For pure states, we simply have \( \delta_{\text{pure}} = \text{Tr}(V^{-1}dVV^{-1}dV) \).

B. Multimode quantum metrology

Let us consider a real parameter \( \theta \) which is encoded in a multimode Gaussian state \( \hat{\rho}_0 \). To estimate \( \theta \) with high precision, it is necessary to distinguish the two infinitesimally-close states \( \hat{\rho}_0 \) and \( \hat{\rho}_{0 + d\theta} \) for an infinitesimal change \( d\theta \). Assume that \( N \) copies of the state \( \hat{\rho}_0 \) are available to an observer, who performs \( N \) independent measurements to obtain an unbiased estimator \( \hat{\theta} \) for parameter \( \theta \). Then, the mean-square error affecting the parameter estimation \( \text{Var}(\hat{\theta}) := \langle (\hat{\theta} - \theta)^2 \rangle \) satisfies the quantum Cramer-Rao (QCR) bound \( \text{Var}(\hat{\theta}) \geq [N\mathcal{H}(\theta)]^{-1} \), where \( \mathcal{H}(\theta) \) is the quantum Fisher information (QFI) \([18]\). The latter can be computed from the fidelity as

\[
\mathcal{H}(\theta) = \frac{8}{d\theta^2} \left[ 1 - \mathcal{F}(\hat{\rho}_0, \hat{\rho}_{0 + d\theta}) \right].
\]

(28)

Thus, for any parametrization of the Gaussian states, we can easily compute the fidelity \( \mathcal{F}(\hat{\rho}_0, \hat{\rho}_{0 + d\theta}) \) using Eq. (9) and, therefore, the QFI in Eq. (28).

More generally, suppose that the Gaussian state is labelled by a vectorial parameter with \( m \) real components, i.e., \( \theta = \{ \theta_i \} \) for \( i = 1, \ldots, m \). In this case, the performance of the parameter estimation is expressed by the classical covariance matrix \( \text{Cov}_{ij}(\theta) := \langle \theta_i\theta_j \rangle - \langle \theta_i \rangle \langle \theta_j \rangle \), which satisfies the matrix version of the QCR bound \([19, 38]\) \( \text{Cov}(\theta) \geq [N\mathcal{H}(\theta)]^{-1} \). Here the QFI is a matrix with elements \( \mathcal{H}_{ij}(\theta) \), which can be evaluated from the Bures metric. In fact, for any parametrization, we may write Eq. (26) as \( ds^2 = g_{ij}(\theta)d\theta_id\theta_j \) and show that \( \mathcal{H}_{ij}(\theta) = 4g_{ij}(\theta) \).

C. Multimode quantum hypothesis testing

An efficient computation of the quantum fidelity is crucial for solving problems of binary quantum hypothesis testing \([30, 31]\) with multimode Gaussian states. These problems
may occur in the basic scenario of quantum state discrimination, where two Gaussian states must be optimally distinguished, or in the setting of quantum channel discrimination, where two Gaussian channels must be distinguished by assuming Gaussian sources and input energy constraints. In particular, the latter formulation is very important in a variety of quantum technology protocols, such as remote quantum sensing of targets, i.e., quantum illumination and quantum reading of classical data from optical memories.

Consider \( N \) copies of two multimode Gaussian states, \( \rho_1^{N} \) and \( \rho_2^{N} \), with the same a priori probability. The minimum error probability \( p_{\text{err}}(N) \) in their statistical discrimination is provided by the Helstrom bound, which is typically hard to compute for mixed states. For this reason, one resorts to other computable bounds, such as the quantum Chernoff bounds or fidelity-based bounds. Thanks to our result the latter are now the simplest to compute.

For any number of copies \( N \), we may write

\[
1 - \sqrt{1 - \left[ F(\hat{\rho}_1, \hat{\rho}_2) \right]^N} \leq p_{\text{err}}(N) \leq \frac{1}{2} \left( F(\hat{\rho}_1, \hat{\rho}_2) \right)^N. \tag{29}
\]

In particular, the lower bound in Eq. (29) is the tightest known. Note that Eq. (29) can be derived by using the known result for single copy (\( N = 1 \)) and then applying the multiplicative property of the fidelity under tensor products of density operators, so that \( F(\rho_1^{\otimes N}, \rho_2^{\otimes N}) = F(\rho_1, \rho_2)^N \).

The computation of the quantum fidelity is also important for asymmetric quantum hypothesis testing where the two quantum hypotheses have unbalanced Bayesian costs.

\[ p_{\text{err}}(N) \leq \frac{1}{2} \left( F(\hat{\rho}_1, \hat{\rho}_2) \right)^N. \]

VII. CONCLUSIONS

In this work we have solved a long-standing open problem in continuous variable quantum information by deriving a simple computable formula for the quantum fidelity between two arbitrary multimode Gaussian states. Our main formula is expressed in terms of the statistical moments of the Gaussian states, but another formulation is also given in terms of suitable symplectic invariants. By using our formula, one can extend the study of quantum teleportation, cloning, quantum metrology and hypothesis testing well beyond the standard case of two-mode Gaussian states to consider multimode Gaussian resources, with unexplored implications for all these basic quantum information protocols.

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[4] Note that there are two definitions of quantum fidelity in the literature. One is the square-root or Bures fidelity \( F \), which is given by Eq. (8). The other is the Uhlmann-Jozsa fidelity, which is the squared of the previous one, i.e., \( F_{U-J} = F^2 \). Bures fidelity is the direct generalization of the classical fidelity. In fact, if the two density operators commute, we can write \( \rho = \sum_i p_i |\psi_i\rangle \langle \psi_i| \) and \( \sigma = \sum_i q_i |\psi_i\rangle \langle \psi_i| \) for an orthonormal basis \( \{ |\psi_i\rangle \} \). Then, we have \( F_{B}(\rho, \sigma) = \sqrt{\operatorname{Tr}(\rho \sigma)} \), which is the classical fidelity \( F(\rho, \sigma) \) between the two probability distributions \( p_i \) and \( q_i \).
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Appendices

Appendix A: Exponential formula for Gaussian states

Here we show the formulae in Eqs. (5)–(7). The first step is to introduce the symplectic action of a real function $f$ on a CM and how it can be computed in terms of standard matrix functions when $f$ is odd. After this preliminary step, we start by noting that, for thermal states (having $V = D \oplus D$), we can easily write Eq. (5) with $u = 0$ and

$$G = g(D) \oplus g(D), \quad g(v) = 2 \coth^{-1}(2v). \quad (A1)$$

Then, we generalize the formula to zero-mean Gaussian states with arbitrary CMs by noting that $\Omega Q \Omega^T$ transforms as $V$ under symplectic coordinate transformations $Q^* = S Q$. This property allows us to use the symplectic action $g(v)$ which leads to Eq. (6). Finally, we include displacements to extend the result to arbitrary mean values and we compute the normalization factor.

1. Symplectic action and its computation

Then, let $f : \mathbb{R} \to \mathbb{R}$ be a function. The symplectic action $f_*$ on the CM $V$ is defined by [29]

$$f_*(V) = S [f(D) \oplus f(D)] S^T, \quad (A2)$$

where $f(D) = \text{diag}[f(v_1), f(v_2), \ldots, f(v_n)]$ acts as a standard matrix function. Here we prove that, if $f$ is an odd function $f(-x) = -f(x)$, then

$$f_*(V) = f([V]\Omega)+\Omega. \quad (A3)$$

Let us start by proving that Eq. (A3) satisfies the identity

$$f_*(S VS^T) = S f_*(V) S^T. \quad (A4)$$

In fact, we have

$$f_*(S VS^T) = f(S VS^T i\Omega)+\Omega = f(S V(i\Omega S^{-1})i\Omega$$

$$S f_*(V i\Omega S^{-1}) i\Omega = S f_*(V) S^T i\Omega = f_*(V) S^T,$$

where we use the basic property $f(S VS^{-1}) = S f(V) S^{-1}$.

Because of Eq. (A4), without loss of generality, we can focus on the case where $V$ is in diagonal Williamson form, i.e.,

$$V = D \oplus D, \quad D = \text{diag}(v_1, v_2, \ldots, v_n),$$

and we assume that $v_i \neq v_j$ for $i \neq j$. One can easily check that the matrix

$$\tilde{V} = (D \oplus D)i\Omega$$

is Hermitian, so it can be cast into the diagonal form by a unitary matrix $U$. It turns out that $U$ is independent on $v_i$ and

$$\tilde{V} = U^\dagger (D \oplus -D)U, \quad (A5)$$

with eigenvalues $\pm v_i$. If $f$ is an odd function, then

$$f(\tilde{V}) = U^\dagger [f(D) \oplus f(-D)] U = U^\dagger [f(D) \oplus -f(D)] U.$$

The latter matrix has the same structure of $\tilde{V}$ in Eq. (A3). Because $U$ is independent on the diagonal elements, then

$$f(\tilde{V}) = [f(D) \oplus f(D)] i\Omega,$$

which gives

$$f([D \oplus D] i\Omega) i\Omega = f(D) \oplus f(D).$$

This is Eq. (A3) up to a symplectic transformation $S$. 


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2. Proof of the exponential formula

Let us now show that the Gibbs exponential formula of Eq. (5) can describe an arbitrary Gaussian state (not just a thermal state). We start by considering a single-mode thermal state $\rho = e^{-g^2/2}$. In this case, we can write

$$
\hat{Z}_\rho = \frac{1}{1 - e^{-g}} \langle a^\dagger a \rangle = -\frac{1}{\hat{Z}} \frac{\partial \hat{Z}}{\partial g} = \frac{1}{e^g - 1}.
$$

(A6)

In our notation, $a = (x + ip)/\sqrt{2}$ so that $a^\dagger a = \frac{x^2 + p^2}{2} - \frac{i}{2}$ and

$$
v(g) := \langle x^2 \rangle = \langle p^2 \rangle = \langle a^\dagger a \rangle + 1/2.
$$

(A7)

Therefore, from Eqs. (A6) and (A7), we derive

$$
v(g) = \frac{1}{2} \coth \frac{g}{2}.
$$

(A8)

In terms of the quadratures, the thermal state reads

$$
\rho = e^{-\frac{1}{2}(x^2 + p^2)},
$$

(A9)

and its normalization is given by

$$
Z_\rho = \hat{Z}_\rho e^{-\frac{g}{2}} = \frac{1}{e^g - e^{-g}} := z(g).
$$

(A10)

Note that the purity is given by

$$
\text{Tr} \hat{\rho}^2 = Z_\rho / Z_\rho'^2 = z(2g)z^{-1}(g) = \tanh(g/2) = \frac{1}{2} v(g)^{-1},
$$

so that the vacuum corresponds to $g \to \infty$ or $v \to 1/2$.

The previous representation of Eq. (A9) can be generalized to a multimode thermal state of $n \geq 1$ bosonic modes. This state has its CM already in the diagonal Williamson form

$$
V = D \oplus D, \quad D = \text{diag}(v_1, \ldots, v_n).
$$

Thanks to the tensor product structure, we can write

$$
\rho = e^{-\frac{1}{2}g^2 G \Omega}.
$$

(A11)

Here $G := \text{diag}(g_1, \ldots, g_n, g_1, \ldots, g_n)$, where the diagonal elements are given by $g_i = g(v_i)$, where

$$
g(v) = 2 \coth^{-1}(2v)
$$

(A12)

is the inverse of the function in Eq. (A8). Compactly, we set

$$
G = g(D) \oplus g(D).
$$

Now, we study how $G$ and $V$ transform under coordinate transformations $Q' = S \Omega$. We have $V' = S VS^T$ and

$$
G' = S^{-T} G S^{-1} = \Omega S \Omega \Omega S^T \Omega.
$$

(A13)

where Eq. (A13) comes from imposing $Q^T G Q = Q'^T G' Q'$ in Eq. (A11). From Eq. (A13), we see that

$$
(\Omega G \Omega) \rightarrow S (\Omega G \Omega) S^T,
$$

i.e., matrices $V$ and $\Omega G \Omega$ transform in the same way under symplectic coordinate transformations. As a result, they can be related by the symplectic action of the function in Eq. (A12).

In fact, for thermal states, we may write

$$
V = D \oplus D, \quad (\Omega G \Omega) = -g(D \oplus D).
$$

Then, for an arbitrary symplectic transformation $S$, we have

$$
\text{Thermal} \quad D \oplus D \quad \rightarrow \quad V = S (D \oplus D) S^T
$$

and

$$
- g(D \oplus D) \quad \rightarrow \quad \Omega G \Omega = S [-g(D \oplus D)] S^T = -g_u(V).
$$

Thus, using the symplectic action $g_u$, defined from Eq. (A12), and its inverse $v_u$, defined from Eq. (A8), we can derive the relations

$$
G = -2 \Omega \coth^{-1}(2V) \Omega = 2 \Omega \coth^{-1}(2V i \Omega),
$$

and

$$
V = \frac{1}{2} \coth u \left( \frac{\Omega G \Omega}{2} \right) = \frac{1}{2} \coth \left( \frac{i \Omega G}{2} \right) i \Omega,
$$

where we also exploit Eq. (A3). These formulae correspond to those in Eq. (6) given in the main text. The additional formula in Eq. (A4) is obtained by considering that $W = -2V i \Omega$.

a. Extension to non-zero mean

The next step is to include the presence of a generally non-zero mean value in the exponential expression of Eq. (A11). For an arbitrary $u \in \mathbb{R}^n$, consider the displacement operator

$$
D(u) = e^{i \Omega u Q}.
$$

which satisfies $D(u)^\dagger = D(-u)$ and $D(u)QD(u)^\dagger = Q + u$. By applying this operator to Eq. (A11), we can generate an arbitrary Gaussian state with non-zero mean

$$
\rho = D(-u) e^{-\frac{1}{2} \Omega u G} D(u) = e^{-\frac{1}{2} \Omega (Q - u) G (Q - u)}.
$$

(A14)

This is easy to double check. Let us set

$$
\rho = D(-u) \rho_G D(u), \quad \rho_G := e^{-\frac{1}{2} \Omega G G}.
$$

First note that $Z_\rho = Z_{\rho_G}$. Then, we can verify that

$$
\text{Tr} \left[ Q e^{-\frac{1}{2} \Omega (Q - u) G (Q - u)} Z_{\rho_G} \right] = \text{Tr} \left[ Q D(-u) e^{-\frac{1}{2} \Omega u G} D(u) \right] = \text{Tr} \left[ D(u) Q D(-u) e^{-\frac{1}{2} \Omega u G} D(u) \right] = \text{Tr} \left[ (Q + u) e^{-\frac{1}{2} \Omega G G} Z_{\rho_G} \right] = u,
$$

i.e. $\langle Q \rangle = u$. Similarly, $V_{ij} = \frac{1}{2} \langle (Q_i - u_i, Q_j - u_j) \rangle$. 

b. Normalization factor

The trace of an unnormalized Gaussian state $\rho$ is written in Eq. (A6) via the function $z(g) = 1/(e^{g/2} - e^{-g/2})$ defined in Eq. (A10). When $G$ is diagonal (i.e. $V$ is diagonal) then

$$Z_p = \prod_j z(g_j). \quad (A14)$$

Now we write Eq. (A14) in a coordinate independent form. A generic $G$ can be obtained from a diagonal $\tilde{G}$ via a symplectic coordinate transformation, because of the property (A2) of the symplectic action, and because det $S = 1$, one has

$$Z_p = \sqrt{\text{det}(Z_s(G))} = \text{det}(z(G\Omega)i\Omega)^{1/2} = \text{det}(e^{G\Omega/2} - e^{-G\Omega/2})i\Omega^{-1/2}.$$ 

Moreover, $z(g(v)) = \sqrt{\nu^2 - \nu}$. It is simple to prove that

$$Z_p = \prod_j z(g(v_j)) = \prod_j \sqrt{V_j^2 - \frac{1}{4}} \quad (A16)$$

$$= \text{det}(V_{\text{diag}} + \Omega/2)^{1/2} \quad (A17)$$

where $V_{\text{diag}} = \text{diag}(v_1, \ldots, v_n,v_1, \ldots, v_n)$. Since a general $V$ can be written as $V = S V_{\text{diag}} S^T$ and det $S = 1$, then

$$Z_p = \text{det} \left( V + \frac{\Omega}{2} \right)^{1/2},$$

where we used the fact that $S\Omega S^T = \Omega$. By replacing $W = -2Vi\Omega$, we also get

$$Z_p = \text{det} \left( I - W \right)^{1/2}.$$

Appendix B: Computations with Gaussian states

1. Product of two Gaussian states with zero mean

Although the product of two Gaussian states can be readily evaluated thanks to the result of [33], in this section we provide a self-consistent proof.

By using the Baker-Campbell-Hausdorff identity, we can write the product of two zero-mean Gaussian states as

$$e^{-\frac{i}{2}(G'G''G)}e^{-\frac{i}{2}G'G'} = e^{-\frac{i}{2}G'G''G}.$$ \tag{B1}

The above identity is a consequence of the algebra

$$\left[ \frac{G'G}{2}, \frac{G''G'}{2} \right] = \frac{i}{2} G' \left( G\Omega G' - G'\Omega G \right) G'\Omega G' = -\frac{G'G''G'}{2}, \quad (B2)$$

where

$$G = -i\Omega J, G' = -i\Omega J', G'' = -i\Omega J''$$

and $J'' = [J, J']$. Because of the above identity, we can write the Eq. (B1) with $e^{G''G'} = e^{e^{G'G}}$, namely

$$e^{-\frac{i}{2}G'G''G} = e^{-\frac{i}{2}G'G}e^{-\frac{i}{2}G'G'}.$$ \tag{B3}

Now we can express the composition rule of Eq. (B3) in terms of the CMs $V$ and $V'$ of the two states $\rho$ and $\rho'$. From Eq. (B4), we have

$$V = \frac{1}{2} e^{G'G} + \frac{1}{2} e^{G''G} \quad (B4)$$

$$= -2Vi\Omega - \frac{1}{2}.$$ 

In terms of $W = -2Vi\Omega, W'$ and $W''$, we may write

$$W'' = -\frac{e^{G'G} G'' + \frac{1}{2}}{e^{G''G} G' + \frac{1}{2}} = \frac{W - I}{W' - \frac{1}{2}} + \frac{W' + \frac{1}{2}}{W'' - \frac{1}{2}}$$

$$= \frac{1}{W' + \frac{1}{2}} + \frac{1}{W'' - \frac{1}{2}}.$$ 

In the above equations, we fix the notation $\frac{1}{2} = AB^{-1}$ when $[A, B] \neq 0$. Using the Woodbury identity [36]

$$(A + B)^{-1} = A^{-1} - A^{-1}(A + B^{-1})^{-1}A^{-1} \quad (B4)$$

we derive

$$W'' = I + (W' + I + (W' + I)^{-1})^{-1}.$$ 

Then, using another straightforward matrix equation

$$W'' = I + (W' + I)(W' + W + I)^{-1}.$$ 

Therefore

$$V'' = -\frac{i}{2} \frac{\Omega}{2} + \left( V' + \frac{i}{2} \right)^{-1} \left( V + \frac{i}{2} \right). \quad (B5)$$

Note that the squared of a Gaussian state $\rho^2$ has $G(2) = 2G$ and its CM can be computed directly from the previous Eqs. (B5) and (B6) by setting $W = W'$ and $V = V'$. It is easy to check that we get

$$V^{(2)} = \frac{1}{2} \left( V + \frac{i}{2} \right)^{-1}, \quad W^{(2)} = \frac{1}{2} \left( W + W^{-1} \right).$$

2. Square root of Gaussian states

Given a Gaussian state $\rho$, its square-root $\sqrt{\rho}$ is a state with $G \rightarrow G/2$. The CM $V_{sq}$ of $\sqrt{\rho}$ can be written in terms of the CM $V$ of $\rho$ by concatenating functions

$$V_{sq}(v) := v(g(v)/2) = \sqrt{1 - \frac{1}{4v^2} + \frac{1}{4}} v. \quad (B7)$$
Notice that, because $v \geq 1/2$ one might be tempted to simplify $v_{sq}(v)$ into the expression $x + \sqrt{4x^2 - 1}/2$. However, the latter function is not odd, so it produces wrong results when it is used for the symplectic action. Eq. (B7) is the correct one. When $V$ is Williamson-diagonal, so it is $V_{sq}$ and the diagonal elements are given by $[V_{sq}]_{ii} = v_{sq}(v)$. Since $V$ and $V_{sq}$ transform in the same way under symplectic transformations, for any general (non-diagonal) $V$, the relation between $V$ and $V_{sq}$ can be obtained with the symplectic action

$$V_{sq} = v_{sq}(V) = \left( \sqrt{\mathbb{I} + \frac{(V\Omega)^2}{4}} + \mathbb{I} \right) V.$$  

By replacing $W = -2\nu i\Omega$, we finally derive

$$W_{sq} = \left( \sqrt{\mathbb{I} - W^{-2} + \mathbb{I}} \right) W.$$  

(B8)

3. Extending the product formula to Gaussian states with non-zero mean

When an operator linear in terms of $Q$ is introduced, the algebra in Eq. (B2) has to be extended. It turns out that

$$\left[ -\frac{1}{2} Q^T G Q , Q \right] = i\Omega G Q ,$$

$$[u^T Q , v^T Q] = u^T i\Omega v.$$  

(B9)

Therefore, $D(u)QD(u)^\dagger = Q+u$, and using Eqs. (B2) and (B9), we may write the identities

$$D(u)D(v) = D(u+v)e^{-i\nu^2/\Omega},$$

$$e^{-\frac{1}{2} Q^T G Q} e^{\frac{i}{2} Q^T G Q} = e^{i\Omega G} Q.$$  

(B10)

4. Decomposition of displaced Gaussian states

Using the previous identities we may write

$$\rho = e^{-\frac{1}{2} (Q-u)^T G (Q-u)} = e^{-\frac{1}{2} \nu^2 \Omega} e^{-\frac{1}{2} Q^T G Q} e^{i\nu^2/\Omega},$$

$$= e^{-\frac{1}{2} \nu^2 \Omega} e^{i\nu^2/\Omega} e^{-\frac{1}{2} Q^T G Q},$$

$$= e^{-\frac{1}{2} \nu^2 \Omega} e^{i\nu^2/\Omega} e^{-i\nu^2/\Omega} e^{-\frac{1}{2} Q^T G Q},$$

$$= e^{\frac{1}{2} \nu^2 \Omega} e^{i\nu^2/\Omega} e^{-\frac{1}{2} Q^T G Q}.$$  

Let $\ell = e^{-i\Omega G} u - u$, i.e.

$$u = (e^{-i\Omega G} - \mathbb{I})^{-1} \ell.$$  

Note that

$$u^T i\Omega e^{-i\Omega G} u = \mathbb{R}[u^T i\Omega e^{-i\Omega G} u]$$

$$= \frac{1}{2} u^T i\Omega (e^{-i\Omega G} - e^{i\Omega G}) u.$$  

(B11)

Then, using the above result

$$e^{i\ell^T G Q} e^{-i\frac{1}{2} \Omega^T G Q} e^{i\frac{1}{2} (Q-u)^T G (Q-u)} e^{i\nu^2/\Omega} = \rho(G, u) e^{-K},$$  

(B12)

where

$$K = \frac{1}{4} u^T i\Omega (e^{-i\Omega G} - e^{i\Omega G}) u$$

$$= \frac{1}{4} i\Omega (e^{i\Omega G} - \mathbb{I})^{-1} i\Omega (e^{-i\Omega G} - e^{i\Omega G} - \mathbb{I})^{-1} \ell$$

$$= \frac{1}{4} i\Omega (e^{i\Omega G} - \mathbb{I})^{-1} (e^{-i\Omega G} - e^{i\Omega G} - \mathbb{I})^{-1} \ell$$

$$= \frac{1}{4} i\Omega \left( -\frac{W + \mathbb{I}}{2} - \frac{W - \mathbb{I}}{2} \right) \ell$$

$$= -\frac{1}{4} i\Omega W \ell.$$  

Appendix C: Proof of Eq. (9)

We start by considering the undisplaced case where $u_1 = u_2 = 0$. This assumption will be relaxed in Appendix C5.

The total state $\rho_{tot} := \sqrt{\nu} \rho_1 \sqrt{\nu}$ has CM $V_{tot} (W_{tot})$ and its Gibbs matrix $G_{tot}$ can be derived by applying the composition rule of Eq. (B3) and noting that $\sqrt{\nu}$ has G/2. Thus, we have

$$\exp(i\Omega G_{tot}) = \exp\left(\frac{i\Omega G_1}{2}\right) \exp\left(i\Omega G_2\right) \exp\left(\frac{i\Omega G_1}{2}\right).$$  

(C1)

Using the expression of the partition function $Z_\nu$ in Eq. (5), the relation between the CM $V$ and the Gibbs matrix in Eq. (6) into $F(\hat{\rho}_1, \hat{\rho}_2) = Z(\sqrt{\nu})/Z(\sqrt{\nu})$, we may write

$$F(\hat{\rho}_1, \hat{\rho}_2) = \frac{\det(e^{i\Omega G_{tot}/4} - e^{-i\Omega G_{tot}/4}) \det(e^{i\Omega G_{tot}/4} - e^{-i\Omega G_{tot}/4})}{\det(e^{i\Omega G_{tot}/2} - e^{-i\Omega G_{tot}/2}) \det(e^{i\Omega G_{tot}/2} - e^{-i\Omega G_{tot}/2})}$$

$$= \frac{\det(e^{i\Omega G_{tot}/2} - \mathbb{I}) \det(e^{i\Omega G_{tot}/2} - \mathbb{I})}{\det(e^{i\Omega G_{tot}/2} - \mathbb{I}) \det(e^{i\Omega G_{tot}/2} - \mathbb{I})}$$

$$= \frac{\det(e^{i\Omega G_{tot}/2} - \mathbb{I}) \det(e^{i\Omega G_{tot}/2} + \mathbb{I})}{\det(e^{i\Omega G_{tot}/2} - \mathbb{I}) \det(e^{i\Omega G_{tot}/2} + \mathbb{I})}$$

$$= \left[ \Gamma(G_1, G_2) F_{tot} \right]^{-4}$$  

(C2)

where

$$\Gamma(G_1, G_2) := 4 \frac{\det(\mathbb{I} - e^{-i\Omega G_1}) \det(e^{i\Omega G_2} - \mathbb{I})}{\det(e^{i\Omega G_1} - e^{-i\Omega G_1}) \det(\Omega)},$$

$$F_{tot} := \frac{\det(e^{i\Omega G_{tot}/2} + \mathbb{I})}{\det(e^{i\Omega G_{tot}/2} - \mathbb{I})} \det i\Omega.$$  

(C3)
Now it is easy to check that
\[ \Gamma(G_1, G_2) = \frac{1}{\sqrt{|\det(V_1 + V_2)|}}. \]  
(C4)

By contrast, the computation of \( F_{\text{tot}} \) is more difficult. Using Eq. (7) we may write \( F_{\text{tot}} \) in terms of \( V_{\text{tot}} \) as follows
\[ F_{\text{tot}} = \det \left[ \left( \sqrt{I - W_{\text{tot}}^{-2}} + I \right) W_{\text{tot}} \right]^{1/4}, \]  
(C5)
or, equivalently, in terms of \( V_{\text{tot}} \) as follows
\[ F_{\text{tot}} = \det \left[ \left( \sqrt{1 + \frac{(V_{\text{tot}} + \Omega)^2}{4}} + I \right) V_{\text{tot}} \right]^{1/4}. \]  
(C6)

Let us compute \( W_{\text{tot}} \) as a function of \( W_1 \) and \( W_2 \). For this we iterate the composition rule in Eq. (B5) and we use the following relations for the \( W \)-matrix of the square-root state
\[ W_{\text{sq}} = \left( \sqrt{I - W_{\text{sq}}^{-2}} + I \right) W, \]  
(C7)
\[ W = \frac{1}{2} \left( W_{\text{sq}} + W_{\text{sq}}^{-1} \right). \]  
(C8)

Let us start by applying Eq. (B5) twice. We have
\[ W'' = I + (W_2 - I)(W_{\text{sq}} + W_2)^{-1}(W_{\text{sq}} - I), \]
\[ W_{\text{tot}} = I + (W_{\text{sq}} - I)(W_{\text{sq}} + W''^{-1}(W'' - I) = I + (W_{\text{sq}} - I)(W_{\text{sq}} + W''^{-1}) \times \]
\[ (W_2 - I)(W_{\text{sq}} + W_2)^{-1}(W_{\text{sq}} - I). \]

Now the next step is to apply the Woodbury identity and \((A^{-1} + B^{-1})^{-1} = A(A + B)^{-1}B\) multiple times, so that we have
\[ [W_{\text{sq}} + I + (W_2 - I)(W_{\text{sq}} + W_2)^{-1}(W_{\text{sq}} - I)]^{-1} = \]
\[ (W_{\text{sq}} - I)\left( (W_{\text{sq}} + W_2)^{-1} + \frac{I}{W_2 - I} W_{\text{sq}} - I \right)^{-1} \]
\[ (W_{\text{sq}} + W_2)^{-1}(W_{\text{sq}} - I), \]
and we may write
\[ W_{\text{tot}} = I + \left( (W_{\text{sq}} + W_2)^{-1} + \frac{I}{W_2 - I} W_{\text{sq}} - I \right)^{-1} \times \]
\[ (W_{\text{sq}} + W_2)^{-1}(W_{\text{sq}} - I), \]
where
\[ X = W_{\text{sq}} + W_2 + \frac{W_{\text{sq}} - I}{W_{\text{sq}} + I} (W_2 - I) \]
\[ = \frac{W_{\text{sq}} + I}{W_{\text{sq}} + I} (I + W_{\text{sq}}^2 + 2W_{\text{sq}} W_2) \]
\[ = \frac{W_{\text{sq}} - I}{W_{\text{tot}} - I} \left( W_{\text{tot}} + I \right)^2 = \frac{2W_{\text{tot}}}{W_{\text{tot}} + I} (W_1 + W_2), \]
and we have used Eq. (C8). Therefore
\[ W_{\text{tot}} = W_{\text{tot}} - \frac{1}{2} (W_{\text{tot}} + W_2)(W_1 + W_2)^{-1}(W_{\text{tot}} - W_{\text{tot}}^{-1}). \]
Because \( W_{\text{sq}} + W_2 = W_{\text{tot}} + W_2 + W_1 - W_1 \) and \( \frac{1}{2} (W_{\text{tot}} - W_{\text{tot}}^{-1}) = W_{\text{tot}} - W_1 \), we may write
\[ W_{\text{tot}} = W_1 - (W_{\text{tot}} - W_1)(W_1 + W_2)^{-1}(W_{\text{tot}} - W_1). \]

This is already a simple expression, but it can be further simplified. Let us write its inverse
\[ W_{\text{tot}}^{-1} = \frac{I}{W_{\text{tot}} - W_1} \left( \frac{W_1}{W_{\text{tot}} - W_1} - \frac{I}{W_1 + W_2} \right)^{-1} \frac{I}{W_{\text{tot}} - W_1}. \]
Using Eq. (C7) we may write
\[ (W_{\text{tot}} - W_1)^2 = W_1 - W_1^{-1}, \]
which, replaced in the previous expression of \( W_{\text{tot}}^{-1} \), leads to
\[ W_{\text{tot}}^{-1} = \frac{W_{\text{tot}} - W_1}{W_1} \left( W_1 - W_1^{-1} - W_1 - W_2 \right)^{-1} \times (W_1 + W_2) \frac{I}{W_{\text{tot}} - W_1} \]
\[ = -(W_{\text{tot}} - W_1)(W_1 + W_2)^{-1}(W_1 + W_2) \frac{I}{W_{\text{tot}} - W_1} \]
\[ = (W_{\text{tot}} - W_1) W_{\text{aux}}^{-1} \frac{I}{W_{\text{tot}} - W_1}, \]  
(C9)
where
\[ W_{\text{aux}} = \frac{I}{W_1 + W_2}(I + W_2 W_1). \]  
(C10)

Because in Eq. (C9) there is a determinant of matrix function, such expression is invariant under \( MWM^{-1} \) transformations (with non-singular \( M \)). Therefore, we can use \( W_{\text{aux}} \) in the place of \( W_{\text{tot}} \) in Eq. (C5). In other words, we may write
\[ F_{\text{tot}} = \det \left[ \left( \sqrt{I - W_{\text{aux}}^{-2}} + I \right) W_{\text{aux}} \right]^{1/4}, \]  
(C11)
\[ = \det \left[ \left( \sqrt{1 + \frac{(V_{\text{aux}} + \Omega)^2}{4}} + I \right) V_{\text{aux}} \right]^{1/4}, \]  
(C12)
where we have used \( W_{\text{aux}} = -2V_{\text{aux}} \Omega \). Combining Eqs. (C2), (C4) and (C12), we obtain Eq. (9), (13) and (14).

1. **Comment for pure states**

The most important result of the previous sections is the similarity transformation which relates \( W_{\text{tot}} \) and \( W_{\text{aux}} \):
\[ W_{\text{tot}} = (W_{\text{tot}} - W_1) W_{\text{aux}} \frac{I}{W_{\text{tot}} - W_1}. \]  
(C13)

However, when \( \rho_1 \) is pure \( W_{\text{tot}} = W_1 \) so the above transformation is singular. The purpose of this section is to show that the final result \( \text{C12} \) is consistent even when the matrix \( W_{\text{tot}} - W_1 \) is singular.
To simplify the notation we assume that $\rho_1$ is a pure state, so the symplectic eigenvalues $\psi_i$ are equal $\psi_i = 1/2$, $\forall i$, although the following argument can be easily generalized to the case in which only few eigenvalues are equal to 1/2. Because Eq. (C5) is basis independent, we perform the calculation in the basis where $W_1$ is diagonal and we write

$$W_1 = \lim_{\epsilon \to 1} W_1(\epsilon), \quad W_1(\epsilon) = \epsilon D_1, \quad D_1 = I \oplus (I \otimes) \quad (C14)$$

Since Eq. (C5) depends only on the eigenvalues of $W_{\text{tot}}$ and the eigenvalues are smooth under perturbations we can write

$$F_{\text{tot}} = \lim_{\epsilon \to 1} \det \left( \sqrt{\frac{1}{\epsilon} - W_{\text{tot}}^{-2}(\epsilon)} + I \right)^{1/4} W_{\text{tot}}(\epsilon) \Omega \right), \quad (C15)$$

where $W_{\text{tot}}(\epsilon)$ refers to $W_{\text{tot}}$ with $W_1$ substituted by $W_1(\epsilon)$. For any $\epsilon < 1$, it is $W_{1\text{sq}} - W_1 = \sqrt{1 - \epsilon^2} D_1$ so the similarity transform of $C13$ is well defined and $C15$ can be replaced by $C11$. Although the matrix $W_{1\text{sq}} - W_1$ is singular for $\epsilon \to 1$ its dependence cancels out, while $W_{\text{aux}}$ is well-defined even in the limit $\epsilon \to 1$.

This is confirmed by the fact that $C5$ reproduces the known results when $\rho_1$ is pure. In the next section we expand this point to simplify the numerical treatment of the singular case.

3. Alternative Formula

Note that in the proof of Sec. C we can exploit the fact that $\det[f(V)] = \det[f(UVU^{-1})]$ for some invertible matrix $U$. By using Eq. (C1) into Eq. (C3), we get

$$F^4_{\text{tot}} = \frac{\det \sqrt{\frac{1}{\epsilon} W_{\text{tot}}^{-2}(\epsilon) + I}}{\det \sqrt{\frac{1}{\epsilon} W_{\text{tot}}^{-2}(\epsilon) - I}} \det i\Omega,$$

and with either $U = e^{\Delta G_i/2}$ or $U = e^{-\Delta G_i/2}$

$$F^4_{\text{tot}} = \frac{\det \sqrt{\frac{1}{\epsilon} W_{\text{tot}}^{-2}(\epsilon) + I}}{\det \sqrt{\frac{1}{\epsilon} W_{\text{tot}}^{-2}(\epsilon) - I}} \det i\Omega. \quad (C18)$$

Finally, after simple algebra, we may write

$$F^4_{\text{tot}} = \det \left( \sqrt{\frac{1}{\epsilon} \frac{V_{12}}{4}} + I \right) V_{12} \quad (C19)$$

$$= \det \left( \sqrt{\frac{1}{\epsilon} \frac{V_{21}}{4}} + I \right) V_{21} \quad (C20)$$

being

$$V_{12} = \frac{-i\Omega}{2} + \left( V + \frac{i\Omega}{2} \right) (V + V_2)^{-1} \left( V_2 + \frac{i\Omega}{2} \right),$$

and $V_{21} = V_{12}^\dagger$. Note that, contrary to matrix $V_{\text{aux}}$, the new matrix $V_{12}$ is not real. Because of the above derivation, $W_{\text{tot}} = e^{\Delta G_i/2} W_{12} e^{-\Delta G_i/2}$, and $W_{\text{tot}} = e^{-\Delta G_i/2} W_{21} e^{\Delta G_i/2}$ so the matrices $W_{\text{tot}}$, $W_{12}$ and $W_{21}$ are similar.

The relation between $V_{12}$ and $V_{\text{aux}}$ is easy to obtain using the $W$ matrices and applying the Woodbury identity. We find

$$W_{12} = I + (W_1 - I)(W_1 + W_2)^{-1}(W_2 - I)$$

$$= (W_1 - I) \left( \frac{I}{W_1 W_2 W_1 - W_1 - W_2 + I} + \frac{I}{W_1 + W_2} \right) (W_2 - I)$$

$$= (W_2 - I)^{-1} \left( \frac{I}{W_1 W_2} (W_1 + W_2) - I \right)$$

$$= (W_1 - I) \frac{I}{W_1 + W_2} (W_2 W_1 + I)(W_1 - I)^{-1} \quad (C21)$$

so that $W_{12} = -U^{-1} W_{\text{aux}} U^{-1}$ for some invertible $U$, as we can see by comparing Eq. (C21) with Eq. (C10).

4. Exchanging $\rho_1$ and $\rho_2$

The final result for the fidelity, Eq. (C11), depends on the matrix $W_{\text{aux}}$ which is not symmetric upon exchanging $\rho_1$ and $\rho_2$. This is due to the apparent asymmetry in the definition of the fidelity. However, we show here that $C11$ is invariant under such exchange, even though $W_{\text{aux}}$ is not. Indeed, thanks to the results of the previous section, if $F(W) =$
det\left[\left(\sqrt{1 - W^2} + \mathbb{I}\right)W\right]^{1/4}, then \(F_{\text{tot}} = F(W_{\text{tot}}) = F(W_{\text{aux}}) = F(W_{12}) = F(W_{21})\). Because \(W_{\text{aux}}\) is similar to \(W_{12}\) (apart from a global sign), which again is similar to \(W_{21}\), if we exchange \(\rho_1\) and \(\rho_2\), the resulting \(W_{\text{aux}}\) (with indices 1 and 2 swapped) is similar to the original one. Therefore, \((C11)\) is invariant under such exchange.

5. Derivation of the fidelity for displaced Gaussian states

Consider displaced Gaussian states, \(\rho_1\) having Gibbs matrix \(G_1\) and mean value \(u_1\), and \(\rho_2\), having \(G_2\) and \(u_2\). Then

\[
\mathcal{F}(\hat{\rho}_1, \hat{\rho}_2) = \frac{Z_{\sqrt{\rho_{\text{tot}}}}}{\sqrt{Z_{\rho_1}Z_{\rho_2}}} = \frac{Z_{\sqrt{\rho_{\text{tot}}}}}{\sqrt{Z_{\rho_1}Z_{\rho_2}}} = \mathcal{F}(\hat{\rho}_{G_1}, \hat{\rho}_{G_2}) \frac{Z_{\sqrt{\rho_{\text{tot}}}}}{Z_{\sqrt{\rho_{\text{tot}}}}},
\]

where \(\mathcal{F}(\hat{\rho}_{G_1}, \hat{\rho}_{G_2})\) is the fidelity (already computed) between two undisplaced Gaussian states, i.e., with Gibbs matrices \(G_1\) and \(G_2\) but zero mean values. Therefore, we only need to compute \(Z_{\sqrt{\rho_{\text{tot}}}}/Z_{\sqrt{\rho_{\text{tot}}}}\).

If we write

\[
\rho_{\text{tot}} = e^{-\frac{1}{2}(Q-u_{\text{tot}})^T G_{\text{tot}} (Q-u_{\text{tot}})} + K_{\text{tot}}
\]

then

\[
Z_{\sqrt{\rho_{\text{tot}}}} = Z_{\sqrt{\rho_{\text{tot}}}}^{K_{\text{tot}}/2}.
\]

Moreover, from the definition one can see that

\[
\mathcal{F}(\hat{\rho}_{G_1}, \hat{\rho}_{G_2}) = \frac{Z_{\rho_1 \rho_2}}{Z_{\rho_1} Z_{\rho_2}}.
\]

For the numerator we may write

\[
Z_{\rho_1 \rho_2} = \text{Tr}[\rho_1 \rho_2] = \text{Tr}[D(-u_1)\rho_{G_1} D(u_1) D(-u_2)\rho_{G_2} D(u_2)]
\]

\[
= \text{Tr}[D(u_2 - u_1) \rho_{G_1} D(u_1 - u_2) \rho_{G_2}]
\]

where the phase in Eq. \((B10)\) vanishes after the twofold use. Then calling

\[
\delta_u = u_2 - u_1,
\]

and calling \(G_{12}\) the matrix such that

\[
e^{-i\Omega G_{12}} = e^{-i\Omega G_1} e^{-i\Omega G_2},
\]

one has

\[
Z_{\rho_1 \rho_2} = \text{Tr}[e^{i\frac{1}{2}(\delta_u Q G_1 + \delta_u Q G_2)} \rho_{G_1} \rho_{G_2}]
\]

\[
= \text{Tr}[e^{i\frac{1}{2}(\delta_u Q G_1 + \delta_u Q G_2)} \rho_{G_1} \rho_{G_2}]
\]

\[
= \text{Tr}[e^{i\frac{1}{2}(\delta_u Q G_1 + \delta_u Q G_2)} \rho_{G_1} \rho_{G_2}]
\]

\[
= \text{Tr}[e^{i\frac{1}{2}(\delta_u Q G_1 + \delta_u Q G_2)} \rho_{G_1} \rho_{G_2}].
\]

Now, by using Eq. \((B12)\) we find

\[
Z_{\rho_1 \rho_2} = e^{i\frac{1}{2}(\delta_u Q G_1 + \delta_u Q G_2)} \text{Tr}[\rho_{G_1} \rho_{G_2}].
\]

By replacing the latter expression into Eq. \((C22)\), we derive

\[
e^{iK_{\text{tot}}} = e^{i\frac{1}{2}(\delta_u Q G_1 + \delta_u Q G_2)} \text{Tr}[\rho_{G_1} \rho_{G_2}]
\]

\[
= e^{i\frac{1}{2}(\delta_u Q G_1 + \delta_u Q G_2)} \text{Tr}[\rho_{G_1} \rho_{G_2}]
\]

\[
= e^{i\frac{1}{2}(\delta_u Q G_1 + \delta_u Q G_2)} e^{i\frac{1}{2}(\delta_u Q G_1 + \delta_u Q G_2)} \text{Tr}[\rho_{G_1} \rho_{G_2}].
\]

The term \(K_{\text{tot}}\) can be simplified noting that

\[
e^{-i\Omega G_1} - e^{-i\Omega G_2} = \frac{W_1 + \mathbb{I}}{W_1 - \mathbb{I}} - \frac{W_1 - \mathbb{I}}{W_1 + \mathbb{I}} = \frac{4W_1}{W_1^2 - 1},
\]

\[
(1 - e^{-i\Omega G_1}) W_{12} (1 - e^{-i\Omega G_2}) = \frac{2}{W_1 + \mathbb{I}} W_{12} \frac{2}{W_1 - \mathbb{I}}.
\]

and \(W_{12} = \mathbb{I} + W_1 - \mathbb{I} - (W_1 + \mathbb{I})(W_1 + W_2)^{-1}(W_1 - \mathbb{I}),\) which is a consequence of the identity \((B4)\). Therefore, we may write

\[
K_{\text{tot}} = \delta_u T \Omega W_1 + W_2) \delta_u = -\frac{1}{2} \delta_u T (V_1 + V_2) \delta_u,
\]

and finally

\[
\mathcal{F}(\hat{\rho}_1, \hat{\rho}_2) = \frac{F_{\text{tot}}}{(\det(V_1 + V_2))^{1/4}} e^{-\frac{1}{2}\delta_u T (V_1 + V_2) \delta_u}.
\]

Appendix D: Proof that the solutions for the three-mode case are real

As written in \((23)\), in the three-mode case the characteristic polynomial \((16)\) can be written as \(\chi = p^3 + pt + q\). The equation \(\chi = 0\) has real solutions if \(p < 0\) and \(q^2/4 + p^3/27 < 0\), which is simple to prove. Indeed, calling \(\pm p_{\text{aux}}^3\) the eigenvalues of \(W_{\text{aux}}\) one finds that \(I_{2n} = 2[(w_{\text{aux}}^1)^2n + (w_{\text{aux}}^2)^2n + (w_{\text{aux}}^3)^2n]\). Hence

\[
p = \frac{1}{3}[(w_{\text{aux}}^1)^4 + (w_{\text{aux}}^2)^4 + (w_{\text{aux}}^3)^4]
\]

\[
- (w_{\text{aux}}^1)^2 (w_{\text{aux}}^2)^2 - (w_{\text{aux}}^1)^2 (w_{\text{aux}}^3)^2 - (w_{\text{aux}}^2)^2 (w_{\text{aux}}^3)^2
\]

\[
= -\frac{1}{6} \left[(w_{\text{aux}}^1)^2 - (w_{\text{aux}}^2)^2\right]^2 + \left[(w_{\text{aux}}^1)^2 - (w_{\text{aux}}^3)^2\right]^2
\]

\[
+ \left[(w_{\text{aux}}^2)^2 - (w_{\text{aux}}^3)^2\right] \leq 0.
\]

(D1)

Similarly,

\[
\frac{\hat{q}^2}{4} + \frac{\hat{p}^3}{27} = -\frac{1}{108} \left[(w_{\text{aux}}^1)^2 - (w_{\text{aux}}^2)^2\right]\left[(w_{\text{aux}}^1)^2 - (w_{\text{aux}}^3)^2\right]
\]

\[
(w_{\text{aux}}^2)^2 - (w_{\text{aux}}^3)^2 \leq 0.
\]

(D2)

Hence, the eigenvalues of \(W_{\text{aux}}\) are real. The real solutions of \(\chi = 0\) are given by \((24)\).

Appendix E: Derivation of the Bures metric

Let us consider two infinitiesmally-close Gaussian states \(\hat{\rho}_1 = \hat{\rho} \) and \(\hat{\rho}_2 = \hat{\rho} + \tilde{d} \hat{\rho} \). The first state is parametrized by \(G\)
(or $V$) and $u$, while the second state is parametrized by $G + dG$
(or $V + dV$) and $u + du$. Hence, up to the second order

\[
\frac{1}{V_1 + V_2} = \frac{1}{2V} \frac{1}{1 + \frac{dV}{2V}} \approx \frac{1}{2V} \left( 1 - \frac{dV}{2V} + \frac{d^2V}{2V^2} \right),
\]

and

\[
\delta^a_0 (V_1 + V_2)^{-1} \delta_a = du^T V^{-1} du / 2.
\]

In a similar way, we find

\[
-W_{\text{aux}}^{-1} = \frac{1}{2} \frac{1 + W^2 + dW W}{1 + W^2} (2W + dW)
\]

\[
= \frac{2W}{1 + W^2} \frac{1}{1 + W^2} dW W^2 - 1 + 1 + W^2 + dW W^2 - 1
\]

\[
+ \frac{1}{1 + W^2} dW W + dW W^2 - 1 + W^2
\]

Since the fidelity is an invariant, one can perform the calculations in the basis in which $W$ is diagonal. Let us call $\tilde{W}$ the (diagonal) matrix $W$ in this basis and $d\tilde{W}$ the corresponding infinitesimal variation (non-diagonal). Then

\[
- (W_{\text{aux}}^{-1})_{ij} = \frac{2w_i}{1 + w_i^2} \delta_{ij} - \frac{1}{1 + w_i} d\tilde{W}_{ij} w^2_i - 1 + \frac{1}{1 + w_j} d\tilde{W}_{ij} w^2_j - 1
\]

\[
+ \sum_k \frac{1}{1 + w_k} d\tilde{W}_{ik} d\tilde{W}_{kj} w_k w_j - 1
\]

To expand the expression

\[
F_{\text{inf}} = \frac{F_{\text{tot}}}{\det(V_1 + V_2)}
\]

\[
= \frac{\det W_{\text{aux}}}{\det(W + dW/2)} \det \left( \sqrt{I - W_{\text{aux}}^{-1} + I} \right),
\]

one has to expand

\[
\sqrt{I - W_{\text{aux}}^{-1} = K^{(0)} + K^{(1)} + K^{(2)}}
\]

in terms of the $0^{\text{th}}$ order, first order and second order operators $K^{(n)}$. Taking the square of Eq. (E2) and calling

\[
W_{\text{aux}}^{-1} = V^{(0)} + V^{(1)} + V^{(2)}
\]

the $2^{\text{nd}}$ order expansion of $W_{\text{aux}}^{-1}$, we find the relations

\[
K^{(0)}(1) = \frac{1}{2} + V^{(0)}
\]

\[
K^{(1)}(1) + K^{(0)}(2) = -V^{(1)}(V^{(0)} - V^{(0)} V^{(1)}
\]

\[
K^{(1)}(2) + K^{(0)}(1) = -V^{(2)}(V^{(0)} - V^{(0)} V^{(2)} - V^{(1)^2} - K^{(2)}
\]

These explicit calculation of $K^{(n)}$ is long but straightforward. Once the operators $K$ are known, from the expansion

\[
\det(I + X) = e^{Tr \log(1 + X)} \approx e^{Tr[X - Tr(X^2)]/2}
\]

of the three terms in Eq. (E1), we find

\[
F_{\text{inf}} = \exp \left( \frac{1}{4} \sum_{ij} \frac{d\tilde{W}_{ij} d\tilde{W}_{ij}}{1 - w_i w_j} \right),
\]

i.e.

\[
\mathcal{F}(\rho, \rho + d\rho) = \exp \left( -\frac{1}{8} du^T V^{-1} du + \frac{1}{16} \sum_{ij} \frac{d\tilde{W}_{ij} d\tilde{W}_{ij}}{1 - w_i w_j} \right).
\]

The Bures metric is then given by

\[
ds^2 = \frac{1}{4} du^T V^{-1} du + \frac{1}{8} \sum_{ij} \frac{d\tilde{W}_{ij} d\tilde{W}_{ij}}{w_i w_j - 1}.
\]

The above expression can be cast into a basis-independent form by defining the super-operator

\[
\mathcal{L}_A X = AXA.
\]

Indeed

\[
\sum_{ij} \frac{d\tilde{W}_{ij} d\tilde{W}_{ij}}{w_i w_j - 1} = \text{Tr} \left[ \frac{d\tilde{W}}{L - 1} \right]
\]

\[
= \text{Tr} \left[ \frac{dW}{L - 1} \right]
\]

\[
= -4 \text{Tr} \left[ dV \Omega \frac{1}{L - 1} (dV \Omega) \right].
\]

Using

\[
\mathcal{L}_W(dV \Omega) = -4V \Omega dV \Omega \Omega = -4(L \Omega L \Omega dV \Omega),
\]

we find

\[
\sum_{ij} \frac{d\tilde{W}_{ij} d\tilde{W}_{ij}}{w_i w_j - 1} = 4 \text{Tr} \left[ dV \Omega \frac{1}{4L \Omega L \Omega + 1} (dV \Omega) \right]
\]

\[
= 4 \text{Tr} \left[ dV \Omega \frac{1}{4L \Omega + 1} (dV) \right]
\]

\[
= 4 \text{Tr} \left[ dV \frac{1}{4L \Omega + 1} (dV \Omega) \right],
\]

where we have used $L^2 = 1$. Finally, we may write

\[
ds^2 = \frac{1}{4} du^T V^{-1} du + \frac{1}{2} \text{Tr} \left[ dV \Omega \frac{1}{4L \Omega + 1} (dV) \right].
\]

1. Singular case

In the singular case, i.e. when some of the eigenvalues of $W$ are $\pm 1$, the sum in (E2) is performed only along the elements where $w_i w_j \neq 1$. The proof of this fact closely follows an analogous observation in the fermionic case [24]. Let $W = \sum_i w_i |i\rangle \langle i|$ be the eigenvalue decomposition of $W$, where $|i\rangle$ is the eigenvector of $W$ with eigenvalue $w_i$ and let $c_i = w_i^{-1} \in [-1, 1]$, $c_j = \tanh(g_i / 2)$, where $g_i$ are the symplectic eigenvalues of $G$. Using this notation, $dW =
\[ \sum_i (1 - w^2_i) d^i |j\rangle \langle i| + w_i (|i\rangle \langle d^i| + |d^i\rangle \langle i|) \]. Inserting the above expression in (27) we find

\[ \delta := \text{Tr} \left[ dW \frac{1}{L_W} dW \right] \]

\[ = \frac{1}{4} \sum_i (1 - w^2_i) dg_i^2 + \sum_{i \neq j} \frac{(w_i - w_j)^2}{1 - w_i w_j} |\langle d^i| j\rangle|^2. \]

The first term in the above equation is well-defined also when \( w_i \to \pm 1 \). To prove that the second term is bounded we define \( f(x, y) = (x - y)^2 (1 - xy)^{-1} \) and write

\[ \delta = \frac{1}{4} \sum_i (1 - w^2_i) dg_i^2 + \sum_{i \neq j} f(c_i, c_j) w_i w_j |\langle d^i| j\rangle|^2. \]  \hspace{1cm} (E3)

As shown in Lemma 3 of Ref. [24], the function \( f(x, y) \) is bounded in \([-1, 1]^2\), \( f(x, y) \leq 4 \), and \( \lim_{(x, y) \to (\pm 1, \pm 1)} f(x, y) = 0 \). Therefore, the elements such that \( w_i w_j = 1 \) do not contribute in the sum (E3). Numerically, this corresponds to taking the pseudo-inverse of the superoperator in (27) or, equivalently, in manually avoiding the sum over the elements such that \( w_i w_j = 1 \). Therefore, even though Eq. (E3) has been found assuming that \( w_i \neq \pm 1 \), it can be analytically extended to the general case.

Notice that for pure states, where \( w_j = \pm 1 \), the effect of the function \( f \) in (E3) can be obtained equivalently by the function \( \tilde{f}(x, y) = (x - y)^2 / 2 \). Taking this substitution in (E3) we find

\[ \delta_{\text{pure}} = \sum_{i \neq j} \tilde{f}(c_i, c_j) w_i w_j |\langle d^i| j\rangle|^2 = \sum_{i \neq j} \frac{(w_i - w_j)^2}{2 w_i w_j} |\langle d^i| j\rangle|^2 \]

\[ = \frac{1}{2} \text{Tr} \left[ \frac{d^i}{W} \frac{d^i}{W} dW \right]. \]  \hspace{1cm} (E4)

The above equation provides a simpler expression for the Bures metric for a pure Gaussian state.