Chapter 1

Gaussian States

1.1 Canonical commutation relations

The canonical commutation relations (CCR) are central to almost all standard approaches to the quantization of continuous systems, be they motional degrees of freedom of non-relativistic particles ("first" quantization) or bosonic quantum fields ("second" quantization). Given a finite set of degrees of freedom represented by pairs of self-adjoint canonical operators $\hat{x}_j$ and $\hat{p}_j$, for $j = 1, \ldots, n$, the CCR read

$$[\hat{x}_j, \hat{p}_k] = i\delta_{jk}\hbar \, . \tag{1.1}$$

where Ω is a real, canonical anti-symmetric form (also known as the 'symplectic form', for reasons that will become clear in the following), given by the direct sum of identical 2×2 blocks:

$$\Omega = \bigoplus_{j=1}^{n} \omega \, , \quad \text{with} \quad \omega = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \, . \tag{1.2}$$

Note that the identity operator should be understood on the RHS of Eq. (1.1): the commutators of pairs of canonical operators are proportional to c-numbers, and can hence be represented by a complex-valued, rather than operator valued, matrix $i\Omega$. Also, we shall set $\hbar = 1$ and only reinstate it in dealing with practical cases.

Canonical Commutation Relations (CCR). By defining the vector of canonical operators $\hat{\mathbf{r}} = (\hat{x}_1, \hat{p}_1 \ldots \hat{x}_n, \hat{p}_n)^{\mathsf{T}}$, Eq. (1.1) can be expediently recast as the following geometric, label-free, expression

$$[\hat{\mathbf{r}}, \hat{\mathbf{r}}^{\mathsf{T}}] = i\Omega \, , \tag{1.3}$$

where the commutator of row and column vectors of operators should be taken as an outer product.

Borrowing from the optical and field theoretical terminologies, canonical degrees of freedom are also referred to as 'modes'.

Note that $\Omega = -\Omega^{\mathsf{T}}$ and $\Omega^2 = -\mathbb{1}_{2n}$, where $\mathbb{1}_{2n}$ is the $2n \times 2n$ identity matrix. Also, Ω is a real orthogonal transformation: $\Omega^{\mathsf{T}}\Omega = -\Omega^2 = \mathbb{1}_{2n}$.

Re-ordering the canonical operators as $\hat{\mathbf{r}'} = (\hat{x}_1, \dots \hat{x}_n, \hat{p}_1, \dots, \hat{p}_n)^{\mathsf{T}}$ yields the following equivalent expression of the CCR:

$$[\hat{\mathbf{r}'}, \hat{\mathbf{r}'}^{\mathsf{T}}] = i\Omega' \ , \quad \text{with} \quad \Omega' = \begin{pmatrix} 0_n & \mathbb{1}_n \\ -\mathbb{1}_n & 0_n \end{pmatrix} \tag{1.4}$$

where $\mathbb{1}_n$ and 0_n are, respectively, the $n \times n$ identity and null matrices.

Another relevant, equivalent form to express the CCR is given by considering bosonic annihilation and creation operators a_j and $a_j^\dagger$, defined as

$$a_j = \frac{\hat{x}_j + i\hat{p}_j}{\sqrt{2}} \ . \tag{1.5}$$

It is easy to see that the vector of annihilation and creation operators $\boldsymbol{\alpha} = (a_1, a_1^\dagger, \dots, a_n, a_n^\dagger)^{\mathsf{T}}$ is related to $\hat{\mathbf{r}}$ by the unitary transformation $\bar{U}_n$, given by

$$\bar{U} = \bigoplus_{j=1}^{n} \bar{u} \ , \quad \text{with} \quad \bar{u} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix} \ , \tag{1.6}$$

so that the CCR may be equivalently recast as

$$[\boldsymbol{a}, \boldsymbol{a}^\dagger] = [\bar{U}\hat{\mathbf{r}}, \hat{\mathbf{r}}^\dagger \bar{U}^\dagger] = \bar{U}[\hat{\mathbf{r}}, \hat{\mathbf{r}}^\dagger]\bar{U}^\dagger = i\bar{U}\Omega\bar{U}^\dagger = \Sigma = \bigoplus_{j=1}^{n} \sigma_z \ , \tag{1.7}$$

where σ_z is defined as the standard z Pauli matrix:

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \ . \tag{1.8}$$

Note that the adjoint of a vector of operators has been implicitly defined as the vector obtained by transposing the original one and conjugating each of its operator entries, e.g. $\boldsymbol{a}^\dagger = (a_1^\dagger, a_1, \dots, a_n^\dagger, a_n)$. Also, $\hat{\mathbf{r}}^{\mathsf{T}} = \hat{\mathbf{r}}^\dagger$, since all of its entries are hermitian operators.

Often, and especially in the mathematical physics literature, the CCR are expressed by exponentiating the canonical operators, which has the advantage of making the operators involved bounded:[1]

$$\mathrm{e}^{i(\hat{x}_j - \hat{p}_k)} = \mathrm{e}^{i\hat{x}_j}\mathrm{e}^{-i\hat{p}_k}\mathrm{e}^{-\frac{i}{2}\delta_{jk}} = \mathrm{e}^{-i\hat{p}_k}\mathrm{e}^{i\hat{x}_j}\mathrm{e}^{\frac{i}{2}\delta_{jk}} \ . \tag{1.9}$$

[1] The equivalence between this expression and Eq. (1.1) is a straightforward consequence of the following well known corollary of the Baker-Campbell-Hausdorff formula:

$$\mathrm{e}^{A+B} = \mathrm{e}^{A}\mathrm{e}^{B}\mathrm{e}^{-[A,B]/2} \ ,$$

which holds whenever $[A, B]$ is *central*, that is commutes with both A and B. In this case, which is clearly the CCR one, A, B and their commutator form a closed algebra.

The final phase factors in the previous equation imply the non-commutativity of position and momentum shifts, and are a typical signature of quantum mechanics. Eq. (1.9) may be generalised to consider arbitrary shift operators, also known as Weyl operators in the case of the CCR algebra:

$$\begin{aligned} \mathrm{e}^{i(\mathbf{r}_1+\mathbf{r}_2)^{\mathsf{T}}\Omega\hat{\mathbf{r}}} &= \mathrm{e}^{i\mathbf{r}_1^{\mathsf{T}}\Omega\hat{\mathbf{r}}}\mathrm{e}^{i\mathbf{r}_2^{\mathsf{T}}\Omega\hat{\mathbf{r}}}\mathrm{e}^{[\mathbf{r}_1^{\mathsf{T}}\Omega\hat{\mathbf{r}},\mathbf{r}_2^{\mathsf{T}}\Omega\hat{\mathbf{r}}]/2} = \mathrm{e}^{i\mathbf{r}_1^{\mathsf{T}}\Omega\hat{\mathbf{r}}}\mathrm{e}^{i\mathbf{r}_2^{\mathsf{T}}\Omega\hat{\mathbf{r}}}\mathrm{e}^{-[\mathbf{r}_1^{\mathsf{T}}\Omega\hat{\mathbf{r}},\hat{\mathbf{r}}^{\mathsf{T}}\Omega\mathbf{r}_2]/2} \\ &= \mathrm{e}^{i\mathbf{r}_1^{\mathsf{T}}\Omega\hat{\mathbf{r}}}\mathrm{e}^{i\mathbf{r}_2^{\mathsf{T}}\Omega\hat{\mathbf{r}}}\mathrm{e}^{-\mathbf{r}_1^{\mathsf{T}}\Omega[\hat{\mathbf{r}},\hat{\mathbf{r}}^{\mathsf{T}}]\Omega\mathbf{r}_2/2} = \mathrm{e}^{i\mathbf{r}_1^{\mathsf{T}}\Omega\hat{\mathbf{r}}}\mathrm{e}^{i\mathbf{r}_2^{\mathsf{T}}\Omega\hat{\mathbf{r}}}\mathrm{e}^{-i\mathbf{r}_1^{\mathsf{T}}\Omega^3\mathbf{r}_2/2} \\ &= \mathrm{e}^{i\mathbf{r}_1^{\mathsf{T}}\Omega\hat{\mathbf{r}}}\mathrm{e}^{i\mathbf{r}_2^{\mathsf{T}}\Omega\hat{\mathbf{r}}}\mathrm{e}^{i\mathbf{r}_1^{\mathsf{T}}\Omega\mathbf{r}_2/2} = \mathrm{e}^{i\mathbf{r}_2^{\mathsf{T}}\Omega\hat{\mathbf{r}}}\mathrm{e}^{i\mathbf{r}_1^{\mathsf{T}}\Omega\hat{\mathbf{r}}}\mathrm{e}^{-i\mathbf{r}_1^{\mathsf{T}}\Omega\mathbf{r}_2/2}\,,\ \forall\,\mathbf{r}_1,\mathbf{r}_2\in\mathbb{R}^{2n}\,. \end{aligned} \tag{1.10}$$

So that, in terms of the Weyl operators $\hat{D}_{\mathbf{r}} = \mathrm{e}^{i\mathbf{r}^{\mathsf{T}}\Omega\hat{\mathbf{r}}}$, one has

$$\hat{D}_{\mathbf{r}_1+\mathbf{r}_2} = \hat{D}_{\mathbf{r}_1}\hat{D}_{\mathbf{r}_2}\mathrm{e}^{i\mathbf{r}_1^{\mathsf{T}}\Omega\mathbf{r}_2/2}\,. \tag{1.11}$$

Inspection reveals that the CCR algebra does not allow for a representation through finite dimensional matrices. For instance, by taking the trace of the left and right hand side of equation $[\hat{x}_1,\hat{p}_1] = i\mathbb{1}$ and assuming that the trace of a commutator vanishes, as is always the case in finite dimension, one would get $\mathrm{tr}\mathbb{1} = 0$, which is clearly impossible to satisfy. However, infinite dimensional representations of the CCR algebra do exist. As well known from basic quantum mechanics, one can consider the space of square-integrable functions on the real line $L^2(\mathbb{R}^n)$, and define:

$$\hat{x}_j|f\rangle = x_j f(\mathbf{x})\,, \tag{1.12}$$

$$\hat{p}_j|f\rangle = -i\frac{\mathrm{d}}{\mathrm{d}x_j}f(\mathbf{x})\,,\quad \forall\,|f\rangle\equiv f(\mathbf{x})\in L^2(\mathbb{R}^n)\,, \tag{1.13}$$

with $\mathbf{x} = (x_1,\ldots,x_n)$.

The eigenstates of $\hat{x}_j$ (and $\hat{p}_j$) are not part of $L^2(\mathbb{R}^n)$, although we shall still indicate them in the Dirac notation as $|x_j\rangle$ and $|p_j\rangle$, by which we shall denote linear forms on $L^2(\mathbb{R}^n)$ such that

$$\langle x_j'|f\rangle = \langle f|x_j'\rangle^* = f(x_1\ldots,x_{j-1},x_j',x_{j+1},\ldots,x_n)\in L^2(\mathbb{R}^{n-1})\,, \tag{1.14}$$

$\forall\,|f\rangle\equiv f(\mathbf{x})\in L^2(\mathbb{R}^n)$. For a trace-class operator $\hat{O}$, one can then write

$$\mathrm{Tr}\left[\hat{O}\right] = \int_{-\infty}^{+\infty}\langle x|\hat{O}|x\rangle\,\mathrm{d}x\,. \tag{1.15}$$

1.2 Quadratic Hamiltonians and Gaussian states

we will refer, somewhat loosely, to a quadratic Hamiltonian as a Hamiltonian which can be expressed as a polynomial of order two in the canonical operators. In terms of the vector of operators $\hat{\mathbf{r}}$ defined above, the most general quadratic Hamiltonian operator $\hat{H}$ reads, up to an irrelevant additive constant:

$$\hat{H} = \frac{1}{2}\hat{\mathbf{r}}^{\mathsf{T}}H\hat{\mathbf{r}} + \hat{\mathbf{r}}^{\mathsf{T}}\mathbf{r}\,, \tag{1.16}$$

where $\mathbf{r}$ is a $2n$-dimensional real vector and H a symmetric matrix, known as the Hamiltonian matrix and not to be confused with the Hamiltonian operator $\hat{H}$. The matrix H can be assumed to be symmetric because any anti-symmetric component in it would just add a term proportional to the identity operator, because of the CCR, and would thus amount to adding a constant to the Hamiltonian.

The modelling of quantum dynamics through quadratic Hamiltonians is very common when higher order terms are inconspicuous and negligible, as is often the case for quantum light fields. Besides, quadratic Hamiltonians represent a consistent approximation in other situations of great interest for experiments, such as ion traps, opto-mechanical systems, nano-mechanical oscillators, and a number of other systems. Up to interactions, the 'free', local Hamiltonian of a quantum oscillator, $\hat{x}^2 + \hat{p}^2$ in rescaled units, is obviously quadratic.

The diagonalisation of any quadratic Hamiltonian is a rather straightforward mathematical routine. Because, as we shall see, such a diagonalisation rests on identifying degrees of freedom that are decoupled from each other, systems governed by quadratic Hamiltonians are referred to as "quasi-free" in the quantum field theory literature. Notwithstanding the ease with which their dynamics is solved, such systems still offer a very rich scenario for quantum information theory, where the standard methods used for the analysis of quadratic Hamiltonians become powerful allies.

1.2.1 Gaussian states

Let us define the set of Gaussian states as *all the the ground and thermal states of quadratic Hamiltonians with positive definite Hamiltonian matrix* $H > 0$. The restriction to positive definite Hamiltonian matrices corresponds to considering 'stable' systems – i.e., Hamiltonian operators bounded from below – and make the definition above consistent.

Any Gaussian state ϱ_G may hence be written as

$$\varrho_G = \frac{\mathrm{e}^{-\beta \hat{H}}}{\mathrm{Tr}\left[\mathrm{e}^{-\beta \hat{H}}\right]} , \tag{1.17}$$

with $\beta \in \mathbb{R}^+$ and $\hat{H}$ defined by $\mathbf{r}$ and H as in Eq. (1.16), including the limiting instance

$$\varrho_G = \lim_{\beta \to \infty} \frac{\mathrm{e}^{-\beta \hat{H}}}{\mathrm{Tr}\left[\mathrm{e}^{-\beta \hat{H}}\right]} . \tag{1.18}$$

Clearly, all states of the form (1.17) for finite β are by construction mixed states, while all pure Gaussian states are described by Eq. (1.18).

By the definition above, Gaussian states have been parametrized through the Hamiltonian matrix H, the vector $\mathbf{r}$, whose meaning will become clear shortly, and the parameter β, which is intended to mimic a notation well established

in thermodynamics where it would indicate the inverse temperature (up to the Boltzmann constant).

Let us now obtain the diagonal form of states (1.17) and (1.18). First off, notice that, upon redefining $\mathbf{r}' = -H^{-1}\mathbf{r}$ (always possible, as any positive definite H is invertible), and up to an irrelevant constant, the Hamiltonian $\hat{H}$ is equivalent to

$$\hat{H}' = \frac{1}{2}(\hat{\mathbf{r}} - \mathbf{r}')^{\mathsf{T}} H (\hat{\mathbf{r}} - \mathbf{r}') \,, \tag{1.19}$$

which is an alternative form of the most general quadratic Hamiltonian with positive definite H, where the real vector $\mathbf{r}'$ merely shifts the vector of operators $\hat{\mathbf{r}}$. We can prove that this shift is equivalent to the action of a unitary operator by considering the action of a Weyl operator, introduced in Eq. (1.11), on the vector of operators $\hat{\mathbf{r}}$.

We intend to prove that

$$\mathrm{e}^{-i\mathbf{r}'^{\mathsf{T}}\Omega\hat{\mathbf{r}}}\hat{\mathbf{r}}\mathrm{e}^{i\mathbf{r}'^{\mathsf{T}}\Omega\hat{\mathbf{r}}} = \hat{\mathbf{r}} - \mathbf{r}' \,, \tag{1.20}$$

where it is understood that the same Weyl operator acts on all entries of the vector $\hat{\mathbf{r}}$. To this aim, let us define the vector of operators $\hat{\mathbf{f}}(\mathbf{r}') = \mathrm{e}^{-i\mathbf{r}'^{\mathsf{T}}\Omega\hat{\mathbf{r}}}\hat{\mathbf{r}}\mathrm{e}^{i\mathbf{r}'^{\mathsf{T}}\Omega\hat{\mathbf{r}}}$, for which one has $\hat{\mathbf{f}}(0) = \hat{\mathbf{r}}$, as well as

$$\begin{aligned}
\partial_{r'_j}\hat{f}_k\big|_{\mathbf{r}'=0} &= \Big(\partial_{r'_j}\mathrm{e}^{-i\sum_{lm} r'_l\Omega_{lm}\hat{r}_m}\hat{r}_j\mathrm{e}^{i\sum_{st} r'_s\Omega_{st}\hat{r}_t}\Big)\Big|_{\mathbf{r}'=0} \\
&= -i\sum_m \Omega_{jm}[\hat{r}_m, \hat{r}_k] = \sum_m \Omega_{jm}\Omega_{mk} = -\delta_{jk} \,,
\end{aligned}$$

while all the higher order derivatives of $\hat{f}_j$ are obviously zero. Hence, all the derivatives in zero of the smooth operator valued function $\hat{\mathbf{f}}(\mathbf{r}')$ coincide with the derivatives of the function $\hat{\mathbf{r}} - \mathbf{r}'$, which proves Eq. (1.20).[2] Because of Eq. (1.20), the Weyl operators are also known as shift or displacement operators, typically in the quantum optics literature.

Inserting Eq. (1.20) into (1.19) yields

$$\hat{H}' = \frac{1}{2}(\hat{\mathbf{r}} - \mathbf{r}')^{\mathsf{T}} H (\hat{\mathbf{r}} - \mathbf{r}') = \frac{1}{2}\mathrm{e}^{-i\mathbf{r}'^{\mathsf{T}}\Omega\hat{\mathbf{r}}}\hat{\mathbf{r}}^{\mathsf{T}} H \hat{\mathbf{r}}\mathrm{e}^{i\mathbf{r}'^{\mathsf{T}}\Omega\hat{\mathbf{r}}} \,. \tag{1.21}$$

Up to first order displacement operators, one can hence set the vector $\mathbf{r}'$ in the quadratic Hamiltonian $\hat{H}'$ to zero. The effect of the purely quadratic part $\frac{1}{2}\hat{\mathbf{r}}^{\mathsf{T}} H \hat{\mathbf{r}}$ can be understood by considering the transformations it induces on the vector of operators $\hat{\mathbf{r}}$ in the Heisenberg picture, which will be the focus of the next section.

[2] The same conclusion could have been reached by applying the well known Baker-Campbell-Hausdorff relationship

$$\mathrm{e}^{\hat{X}}\hat{Y}\mathrm{e}^{-\hat{X}} = \hat{Y} + [\hat{X}, \hat{Y}] + \frac{1}{2!}[\hat{X}, [\hat{X}, \hat{Y}]] + \frac{1}{3!}[\hat{X}, [\hat{X}, [\hat{X}, \hat{Y}]]] + \dots \,.$$

1.2.2 The symplectic group of linear canonical transformations

Let us now consider the Heisenberg evolution of the vector of operators $\hat{\mathbf{r}}$ under the dynamics governed by the Hamiltonian $\hat{H} = \frac{1}{2}\hat{\mathbf{r}}^{\mathsf{T}} H \hat{\mathbf{r}}$. One has

$$\begin{aligned}\dot{\hat{r}}_j = i[\hat{H}, \hat{r}_j] &= \frac{i}{2}\sum_{kl}[\hat{r}_k H_{kl}\hat{r}_l, \hat{r}_j] \\ &= \frac{i}{2}\sum_{kl} H_{kl}\left(\hat{r}_k[\hat{r}_l, \hat{r}_j] + [\hat{r}_k, \hat{r}_j]\hat{r}_l\right) = \sum_{kl}\Omega_{jk}H_{kl}\hat{r}_l \ , \end{aligned} \tag{1.22}$$

which can be recast in vector form as

$$\dot{\hat{\mathbf{r}}} = \Omega H \hat{\mathbf{r}} \ . \tag{1.23}$$

The solution to the differential equation (1.23) is straightforward and given by $\hat{\mathbf{r}}(t) = \mathrm{e}^{\Omega H t}\hat{\mathbf{r}}(0)$. Since it represents the action of a unitary operation, the transformation $\mathrm{e}^{\Omega H t}$ must preserve the CCR when applied to the vector $\hat{\mathbf{r}}$, that is

$$i\Omega = [\hat{\mathbf{r}}, \hat{\mathbf{r}}^{\mathsf{T}}] = [\mathrm{e}^{\Omega H t}\hat{\mathbf{r}}, \hat{\mathbf{r}}^{\mathsf{T}}(\mathrm{e}^{\Omega H t})^{\mathsf{T}}] = \mathrm{e}^{\Omega H t}[\hat{\mathbf{r}}, \hat{\mathbf{r}}^{\mathsf{T}}](\mathrm{e}^{\Omega H t})^{\mathsf{T}} = i\mathrm{e}^{\Omega H t}\Omega(\mathrm{e}^{\Omega H t})^{\mathsf{T}} \ . \tag{1.24}$$

The transformation $\mathrm{e}^{\Omega H t}$ must therefore preserve the canonical anti-symmetric form Ω when acting by congruence.[3] This can be restated by claiming that $\mathrm{e}^{\Omega H t}$ belongs to the group of linear canonical transformations, well known from classical Hamiltonian mechanics. This group is also known as the real symplectic group in dimension $2n$, denoted by $Sp_{2n,\mathbb{R}}$ (let us remind the reader that H and Ω are $2n \times 2n$ matrices). The quadratic form Ω, which encodes the commutation relations in our formalism, is also known as the symplectic form, and the symplectic group is defined as the set of transformations that preserve Ω under congruence:

$$S \in Sp_{2n,\mathbb{R}} \quad \Leftrightarrow \quad S\Omega S^{\mathsf{T}} = \Omega \ . \tag{1.25}$$

The group character of such a set is ascertained by noting that its elements must be invertible because their determinant cannot be zero by Binet's theorem, and that $S^{-1}\Omega S^{-1\mathsf{T}} = \Omega$ (the inclusion of the identity matrix and of any product of two elements are obvious).

It is expedient to introduce the shorthand notation $\hat{S}_H$ for operators with purely quadratic generators:

$$\hat{S}_H = \mathrm{e}^{i\hat{\mathbf{r}}^{\mathsf{T}} H \hat{\mathbf{r}}} \ , \tag{1.26}$$

such that our argument above allows one to write

$$\hat{S}_H \hat{\mathbf{r}} \hat{S}_H^{\dagger} = S_H \hat{\mathbf{r}} \ , \tag{1.27}$$

[3] We will refer to the matrix A acting "by congruence" on the quadratic form B to indicate the transformation $B \mapsto ABA^{\mathsf{T}}$. The invertible matrix A will instead be said to act "by similarity" on B when it transforms it according to $B \mapsto ABA^{-1}$.

where $S_H = \mathrm{e}^{\Omega H} \in Sp_{2n,\mathbb{R}}$. Notice that, with respect to the treatment above, the time variable t has been absorbed in the symmetric matrix H. The relationship (1.27) will be used extensively throughout the notes.

1.2.3 Normal modes

The normal mode decomposition, whereby a positive definite quadratic form is split into 'decoupled' degrees of freedom, is instrumental in diagonalising quadratic Hamiltonians, and represents one of the methodological cornerstones of quantum continuous variables. This technique, well established since the early days of classical mechanics, can be summarised in the following statement:

Normal mode decomposition. Given a $2n \times 2n$ positive definite real matrix M, there exists a symplectic transformation $S \in Sp_{2n,\mathbb{R}}$ such that

$$SMS^{\mathsf{T}} = D \quad \text{with} \quad D = \mathrm{diag}(d_1, d_1, \ldots, d_n, d_n)\,, \tag{1.28}$$

with $d_j \in \mathbb{R}^+ \ \forall \ j \in [1, \ldots, n]$.

Proof. Since M is invertible and with strictly positive eigenvalues, a set of real matrices S satisfying Eq. (1.28) may be constructed as $S = D^{1/2} O M^{-1/2}$, for all $O \in O(2n)$. We have to show that a choice of the orthogonal transformation O exists such that this matrix is symplectic, which is equivalent to

$$D^{1/2} O M^{-1/2} \Omega M^{-1/2} O^{\mathsf{T}} D^{1/2} = \Omega\,, \tag{1.29}$$

where we have made use of the symmetry of M and D. Now, the matrix $\Omega' = M^{-1/2} \Omega M^{-1/2}$ is clearly anti-symmetric, and for any $2n \times 2n$ real anti-symmetric matrix there exists an orthogonal transformation $O \in O(2n)$ which puts it in a decoupled canonical form, as per:

$$O \Omega' O^{\mathsf{T}} = \bigoplus_{j=1}^{n} d_j^{-1} \omega\,, \tag{1.30}$$

where ω is the 2×2 antisymmetric block defined in Eq. (1.2) and $d_j \in \mathbb{R} \ \forall$

[3] Equation (1.27) expresses the fact that unitary operators generated by purely second-order Hamiltonians form a projective representation of $Sp_{2n,\mathbb{R}}$, that is a representation up to transformation-dependent phase factors. It turns out that a mapping can be defined where such phase factors are always either -1 or $+1$: Technically, one thus achieves a faithful representation of the *metaplectic* group, a double cover of the symplectic group whose exact definition would go beyond the scope of these lectures. It may however be useful to add that this construction is, somewhat loosely, also referred to as the "metaplectic" representation in the literature.

$j \in [1, \ldots, n]$.[4] Hence, one has:

$$D^{1/2} O M^{-1/2} \Omega M^{-1/2} O^{\mathsf{T}} D^{1/2} = D^{1/2} O \Omega' O^{\mathsf{T}} D^{1/2} = \bigoplus_{j=1}^{n} d_j d_j^{-1} \omega = \Omega \,, \quad (1.31)$$

where D has been set to $\mathrm{diag}(d_1, d_1, \ldots, d_n, d_n)$, as anticipated in Eq. (1.28), thus proving the theorem. Note that the quantities d_j must be strictly positive because M is strictly positive.

The symplectic transformation S that turns a matrix M into its normal form is determined by the linear transformation L that diagonalises the matrix $i\Omega M$ (where the conventional factor i is included because the eigenvalues of ΩM are purely imaginary). This can be seen by taking the converse of the normal mode decomposition (1.28): $M = S^{-1} D S^{\mathsf{T}-1}$, and noticing that

$$i\Omega M = i\Omega S^{-1} D S^{\mathsf{T}-1} = i S^{\mathsf{T}} \Omega D S^{\mathsf{T}-1} = i S^{\mathsf{T}} \bar{U} \left(\bigoplus_{j=1}^{n} d_j \sigma_z \right) \bar{U}^{\dagger} S^{\mathsf{T}-1} \,, \quad (1.32)$$

where $\bar{U} = \bigoplus_{j=1}^{n} \bar{u}$, and

$$\bar{u} = \begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix} \quad (1.33)$$

is the transformation that diagonalises ω: $\bar{u} \omega \bar{u}^{\dagger} = \sigma_z$ (note that this is the very same unitary transformation that appeared in Eq. (1.7) to relate ladder and canonical operators). Eq. (1.32) shows that $i\Omega M$ is always diagonalisable for positive definite M and that, if L is the matrix that diagonalises $i\Omega M$ by similarity (such that $L \Omega M L^{-1}$ is diagonal), then one has $S = \bar{U} L^{\dagger}$ (where we accounted for the fact that transposing a real matrix is the same as conjugating it) for the symplectic transformation S that decomposes M in normal modes by congruence.

Eq. (1.32) also implies that the n quantities $\{d_j, j \in [1, \ldots, n]\}$ are the absolute values of the eigenvalues of $i\Omega M$ (which come in pairs of equal modulus and opposite sign). The d_j's are referred to as the symplectic eigenvalues of the positive definite matrix M, while the normal mode decomposition is also known as "symplectic diagonalisation".

[4] The canonical decomposition of anti-symmetric matrices follows from the diagonalisability of symmetric ones: let A be a real, anti-symmetric, $2n \times 2n$ matrix (even dimension is just imposed to fix ideas and because it applies to our case), then A^2 is symmetric and can be diagonalised as per $O A^2 O^{\mathsf{T}} = B$, with B diagonal and $O \in O(2n)$. Consider then a generic eigenvector $\mathbf{e}_1$ of A^2, with eigenvalue $d_1 \in \mathbb{R}$. The vector $\mathbf{e'}_1 = A\mathbf{e}_1$ is clearly orthogonal to $\mathbf{e}_1$, because A is antisymmetric: $\mathbf{e}_1^{\mathsf{T}} A \mathbf{e}_1 = 0$. Let $\mathbf{v}$ be a generic vector in the linear subspace orthogonal to the space spanned by $\mathbf{e}_1$ and $\mathbf{e'}_1$, then one has

$$\mathbf{v}^{\mathsf{T}} A \mathbf{e_1} = \mathbf{v}^{\mathsf{T}} \mathbf{e'_1} = 0 \quad \text{and} \quad \mathbf{v}^{\mathsf{T}} A \mathbf{e'_1} = \mathbf{v}^{\mathsf{T}} A^2 \mathbf{e_1} = 0 \,,$$

as $\mathbf{e_1}$ is an eigenvalue of A^2 by hypothesis. The equation above shows that any choice of orthogonal basis including $\mathbf{e}_1$ and $\mathbf{e'}_1$ would result in A acting as a diagonal block $d_1 \omega$ in the subspace spanned by $\mathbf{e}_1$ and $\mathbf{e'}_1$. Iterating this argument leads to the canonical decomposition of Eq. (1.30).

Note that, since it preserves the CCR, a symplectic transformation acting on the vector of canonical operators corresponds to defining new canonical degrees of freedom which are linearly related to the original ones. As we shall see in detail in the next section, the normal mode decomposition of a $2n \times 2n$ positive definite quadratic Hamiltonian defines a new set of degrees of freedom which are dynamically decoupled under such a Hamiltonian, and oscillate like free harmonic oscillators. In this instance, the n symplectic eigenvalues correspond to the frequencies of the normal modes (also known as "eigenfrequencies" or "normal" frequencies). Let us emphasise that the normal mode decomposition only holds for positive definite matrices, in that a real symplectic S doing the job could only be constructed as above for such matrices.[5]

1.3 Normal mode decomposition of a Gaussian state

Let us now go back to our definition of the set of a Gaussian state given by Eqs. (1.16), (1.17) and (1.18), in terms of a positive definite Hamiltonian matrix H, a vector of displacements $\mathbf{r}$ and an inverse temperature β. We have already seen how to reduce the vector parameter $\mathbf{r}$ to the action of a unitary Weyl operator. The normal mode decomposition puts us in a position to analyse the role of H as well. In fact, because of the theorem proven in the previous section, one can write

$$H = S_H^{\mathsf{T}} \left(\bigoplus_{j=1}^{n} \omega_j \mathbb{1}_2 \right) S_H \quad \text{for} \quad S_H \in Sp_{2n,\mathbb{R}} \,, \tag{1.34}$$

where S_H is the transpose and inverse of the (not necessarily unique) symplectic transformation that puts H in normal form acting by congruence, which always exists because $H > 0$ by hypothesis, and the ω_j's are the symplectic eigenvalues of H (the frequencies of its normal modes). Eq. (1.34) leads to

$$\hat{\mathbf{r}}^{\mathsf{T}} H \hat{\mathbf{r}} = \hat{\mathbf{r}}^{\mathsf{T}} S_H^{\mathsf{T}} \left(\bigoplus_{j=1}^{n} \omega_j \mathbb{1}_2 \right) S_H \hat{\mathbf{r}} \,. \tag{1.35}$$

But our introduction of the symplectic group was based upon the equivalence between the action of a symplectic transformation on the vector of canonical operators, as in $S^{(H)}\hat{\mathbf{r}}$, and the action of a unitary operator generated by a second-order Hamiltonian. In point of fact, any symplectic transformation S may be decomposed into the product of two matrix exponentials.[6] Therefore, a

[5] Trivially, the decomposition extends to negative definite matrices too, which are equivalent to positive definite up to a minus sign.

[6] Any element of a *compact* Lie group – like, *e.g.*, the unitary group in any finite dimension – may be written as a single matrix exponential. This is equivalent to stating that the exponential map from the algebra of generators into the group is surjective for such groups. However, the symplectic group $Sp_{2n,\mathbb{R}}$ is not compact, and it turns out that some of its elements may only be obtained as the product of two exponentials of generators. We will not elaborate further on this issue, which is rather technical and would call for an extensive and detailed mathematical analysis of the properties of $Sp_{2n,\mathbb{R}}$.

pair of symmetric matrices A and B must exist such that

$$S^{(H)}\hat{\mathbf{r}} = \hat{S}_A \hat{S}_B \hat{\mathbf{r}} \hat{S}_B^\dagger \hat{S}_A^\dagger \,, \tag{1.36}$$

where the operators $\hat{S}_A$ and $\hat{S}_B$, defined as per Eq. (1.26), act by similarity on each entry of $\hat{\mathbf{r}}$. The matrices A and B are not necessarily unique, and satisfy the equality $S^{(H)} = \mathrm{e}^{\Omega A}\mathrm{e}^{\Omega B}$, where $S^{(H)}$ was defined above as the inverse and transpose of the symplectic transformation that brings H into normal form. Although in practice it may not be easy to determine A and B analytically, such matrices always exist for any given Hamiltonian matrix H. Notice that, in the interest of rigour, we were forced to introduce two symplectic generators, ΩA and ΩB, because there exist symplectic transformations which require the product of two matrix exponentials to be expressed. However, we can now simplify our notation by defining the unitary transformation $\hat{S} = \hat{S}_A \hat{S}_B$. Inserting Eq. (1.36) into (1.35) yields

$$\hat{\mathbf{r}}^\mathsf{T} H \hat{\mathbf{r}} = \hat{S}\hat{\mathbf{r}}^\mathsf{T} \left(\bigoplus_{j=1}^{n} \omega_j \mathbb{1}_2 \right) \hat{\mathbf{r}}\, \hat{S}^\dagger \tag{1.37}$$

$$= \hat{S} \left(\sum_{j=1}^{n} \omega_j \left(\hat{x}_j^2 + \hat{p}_j^2 \right) \right) \hat{S}^\dagger \,. \tag{1.38}$$

We have thus shown that *every second-order Hamiltonian with zero displacement and positive definite Hamiltonian matrix is unitarily equivalent to the Hamiltonian of a set of free, non-interacting harmonic oscillators.* From now on, let us denote the free Hamiltonian of mode j with frequency ω_j by the shorthand notation $\hat{H}_{\omega_j}$:

$$\hat{H}_{\omega_j} = \frac{\omega_j}{2} \left(\hat{x}_j^2 + \hat{p}_j^2 \right) \,. \tag{1.39}$$

Putting together Eqs. (1.21) and (1.38), the most general second-order Hamiltonian $\hat{H}$ of Eq. (1.19) with positive definite Hamiltonian matrix H may be recast in the form:

$$\hat{H} = \frac{1}{2}(\hat{\mathbf{r}} - \bar{\mathbf{r}})^\mathsf{T} H (\hat{\mathbf{r}} - \bar{\mathbf{r}}) = \hat{D}_{-\bar{\mathbf{r}}} \hat{S} \left(\sum_{j=1}^{n} \hat{H}_{\omega_j} \right) \hat{S}^\dagger \hat{D}_{\bar{\mathbf{r}}} \,, \tag{1.40}$$

$H = \mathrm{e}^{\Omega A}\mathrm{e}^{\Omega B} \bigoplus_{j=1}^{n} \omega_j \mathbb{1}_2 \mathrm{e}^{-B\Omega}\mathrm{e}^{-A\Omega}$, where $\{\omega_j, j \in [1, \ldots, n]\}$ is the set of (doubly-degenerate) eigenvalues of $|i\Omega H|$.[7]

[7] Note that the $2n^2 + n$ real parameters contained in the $2n \times 2n$ real, positive definite matrix H, have been transferred into the symplectic matrix S, which symplectically diagonalises H, plus the set of n symplectic eigenvalues ω_j's. The number of free parameters has not changed though, as the transformation performing the symplectic diagonalisation of any positive definite matrix is in general ambiguous due to the invariance of the Hamiltonian matrix $\mathbb{1}_2$ under local rotations, which are symplectic. Hence, the number of parameters is still $2n^2 + n$ (a generic symmetric matrix) minus n (due to the invariance that was just mentioned) plus n (the number of symplectic eigenvalues), which is consistent with the previous counting.

The same unitary equivalence carries over to Gaussian states, whose operator form ϱ_G, as defined in Eqs. (1.17) and (1.18), only depends on the second-order Hamiltonian $\hat{H}$. Hence, we have derived the most general expression for a Gaussian state ϱ_G as:

$$\varrho_G = \hat{D}_{-\bar{\mathbf{r}}}\hat{S}\frac{\left(\bigotimes_{j=1}^{n} \mathrm{e}^{-\beta\hat{H}_{\omega_j}}\right)}{\prod_{j=1}^{n}\mathrm{Tr}\left[\mathrm{e}^{-\beta\hat{H}_{\omega_j}}\right]}\hat{S}^\dagger\hat{D}_{\bar{\mathbf{r}}}\,, \quad \beta > 0\,. \tag{1.41}$$

One then just needs to put the free Hamiltonian $\hat{H}_{\omega_j}$ in diagonal form in order to obtain the spectrum of any Gaussian state.

Notice how the direct sum of Hamiltonians Eq. (1.37), in the 'phase space' picture set by the vector of canonical operators $\hat{\mathbf{r}}$, turned into a tensor product in the Hilbert space representation. This trait, due to the linearity of the operations acting on $\hat{\mathbf{r}}$, will be an important ingredient in much of our treatment of Gaussian states and their information properties.

1.4 The Fock basis

As we just saw, the diagonal form of the free oscillator's Hamiltonian $\hat{H}_{\omega_j}$ of Eq. (1.39) determines the spectrum of any Gaussian state. Obtaining such a diagonal form is one of the very first notions dealt with in most basic quantum mechanics courses. Nonetheless, it is such a cornerstone of our theoretical framework that we will take the opportunity to concisely recall it here.

The Hamiltonian $\hat{H}_{\omega_j}$ may be recast as $\hat{H}_{\omega_j} = \omega_j\left(a_j^\dagger a_j + \frac{1}{2}\right)$ in terms of the annihilation and creation operators defined in Eq. (1.5). Because of the CCR, it can be easily shown that, if $|\lambda\rangle_j$ is an eigenstate of $\hat{H}_{\omega_j}$ with generic eigenvalue $\omega_j\lambda$, then $a|\lambda\rangle_j$ is an eigenvector too, with eigenvalue $\omega_j(\lambda-1)$. But since the spectrum of $\hat{H}_{\omega_j}$ must be bounded from below, this implies that a state $|0\rangle_j$ must exist such that $a|0\rangle_j = 0$. Such a state is referred to as the vacuum state, and it is the ground state of $\hat{H}_{\omega_j}$, with eigenvalue $1/2$. It is then easy to show that all other eigenvectors of $\hat{H}_{\omega_j}$ may be obtained by m repeated applications of the creation operator $a_j^\dagger$ on $|0\rangle_j$, and that they have eigenvalues $\omega_j\left(m+\frac{1}{2}\right)$, with $m \in \mathbb{N}$. The normalised eigenstates of $\hat{H}_{\omega_j}$ are known as Fock, or number states, and will be denoted with $\{|m\rangle_j, m \in \mathbb{N}\}$. The operator $a_j^\dagger a_j$ is known as the number operator. Let us summarise the action of creation and annihilation operators in the Fock basis:

$$a_j|m\rangle_j = \sqrt{m}|m-1\rangle_j\,, \tag{1.42}$$

$$a_j^\dagger|m\rangle_j = \sqrt{m+1}|m+1\rangle_j\,, \tag{1.43}$$

$$a_j^\dagger a_j|m\rangle_j = m|m\rangle_j\,. \tag{1.44}$$

For a bosonic quantum field, in the second quantization picture, the number state $|m\rangle_j$ represents the presence of m particles (excitations of the field) in mode j.

We can now make use of Eq. (1.41) to determine the spectrum of a generic Gaussian state ϱ_G and express it in the Fock basis. The normalisation factor is promptly evaluated:

$$\frac{1}{\mathrm{Tr}\left[\mathrm{e}^{-\beta\hat{H}_{\omega_j}}\right]} = \frac{1}{\mathrm{e}^{-\frac{\beta\omega_j}{2}}\sum_{m=0}^{\infty}\mathrm{e}^{-\beta\omega_j m}} = \mathrm{e}^{\frac{\beta\omega_j}{2}} - \mathrm{e}^{-\frac{\beta\omega_j}{2}}\,, \tag{1.45}$$

so that

$$\varrho_G(\beta) = \left(\prod_{j=1}^{n}\left(1-\mathrm{e}^{-\beta\omega_j}\right)\right)\hat{D}^{\dagger}_{\mathbf{r}'}\hat{S}_{J_H}\left(\bigotimes_{j=1}^{n}\left(\sum_{m=0}^{\infty}\mathrm{e}^{-\beta\omega_j m}|m\rangle_{jj}\langle m|\right)\right)\hat{S}^{\dagger}_{J_H}\hat{D}_{\mathbf{r}'}\,. \tag{1.46}$$

The limit of pure states, $\beta \mapsto \infty$, is particularly simple and instructive in this representation:

$$\lim_{\beta\to\infty}\varrho_G(\beta) = \hat{D}^{\dagger}_{\mathbf{r}'}\hat{S}_{J_H}|0\rangle\langle 0|\hat{S}^{\dagger}_{J_H}\hat{D}_{\mathbf{r}'}\,, \tag{1.47}$$

where the shorthand notation $|0\rangle = \bigotimes_{j=1}^{n}|0\rangle_j$ has been introduced to represent the vacuum of the whole field. *All pure Gaussian states are obtained by applying unitary operations generated by quadratic Hamiltonians on the vacuum state.*

Note that the positive parameter β is technically redundant, as it might have been absorbed in the Hamiltonian matrix H and, in particular, in its normal frequencies ω_j, as apparent from Eq. (1.46). We have preferred to render it explicit in our treatment because it allows for a very clear definition of the set of pure Gaussian states, and because it relates our formalism to a physical interpretation: the Gaussian state with parameters H, $\mathbf{r}$ and β is the equilibrium state of a system with local quadratic Hamiltonian $\hat{H}$ after thermalisation with a reservoir at rescaled temperature $1/\beta$. In the next section, we will move on to yet another equivalent parametrisation of a generic Gaussian state.

1.5 Statistical moments of a Gaussian state and the covariance matrix

Before proceeding, let us drop the dependence on the quadratic Hamiltonian $\hat{H}$ and assume instead the parametrisation of the most general n-mode Gaussian state, given by Eq. (1.46), in terms of a generic symplectic transformation S, represented in the Hilbert space by $\hat{S}$, of an arbitrary displacement operator $\hat{D}_{\mathbf{r}}$, and of a set of n strictly positive real numbers ξ_j (each replacing $\beta\omega_j$ above). The limit of pure states may still be taken by sending all the ξ_j to infinity. Then one has, for the most general Gaussian state ϱ_G:

$$\varrho_G = \left(\prod_{j=1}^{n}\left(1-\mathrm{e}^{-\xi_j}\right)\right)\hat{D}^{\dagger}_{\mathbf{r}}\hat{S}^{\dagger}\left(\bigotimes_{j=1}^{n}\left(\sum_{m=0}^{\infty}\mathrm{e}^{-\xi_j m}|m\rangle_{jj}\langle m|\right)\right)\hat{S}\hat{D}_{\mathbf{r}}\,. \tag{1.48}$$

Also note that, by virtue of Eqs. (1.20) and (1.36), one has

$$\hat{D}_{\mathbf{r}}\hat{\mathbf{r}}\hat{D}_{\mathbf{r}}^{\dagger} = \hat{\mathbf{r}} + \mathbf{r}\,, \tag{1.49}$$

$$\hat{S}\hat{\mathbf{r}}\hat{S}^{\dagger} = S\hat{\mathbf{r}}\,, \tag{1.50}$$

which express the fact that Weyl operators and unitary operators generated by Hamiltonians of order two projectively represent, respectively, the abelian group of translations in dimension $2d$ and the real symplectic group.

Let us now evaluate the expectation value of $\hat{\mathbf{r}}$ for the Gaussian state ϱ_G:

$$\begin{aligned}
\mathrm{Tr}\left[\varrho_G\hat{\mathbf{r}}\right] &= \prod_{j=1}^{n}\left(1-\mathrm{e}^{-\xi_j}\right)\mathrm{Tr}\left[\left(\bigotimes_{j=1}^{n}\left(\sum_{m=0}^{\infty}\mathrm{e}^{-\xi_j m}|m\rangle_{jj}\langle m|\right)\right)\hat{S}\hat{D}_{\mathbf{r}}\hat{\mathbf{r}}\hat{D}_{\mathbf{r}}^{\dagger}\hat{S}^{\dagger}\right] \\
&= \prod_{j=1}^{n}\left(1-\mathrm{e}^{-\xi_j}\right)\mathrm{Tr}\left[\bigotimes_{j=1}^{n}\left(\sum_{m=0}^{\infty}\mathrm{e}^{-\xi_j m}|m\rangle_{jj}\langle m|\right)(S\hat{\mathbf{r}}+\mathbf{r})\right] \\
&= \prod_{j=1}^{n}\left(1-\mathrm{e}^{-\xi_j}\right)\mathrm{Tr}\left[\bigotimes_{j=1}^{n}\left(\sum_{m=0}^{\infty}\mathrm{e}^{-\xi_j m}|m\rangle_{jj}\langle m|\right)\mathbf{r}\right] = \mathbf{r}\,,
\end{aligned} \tag{1.51}$$

where we used the fact that the expectation value of any linear combination of canonical operators vanishes when calculated on a state which is diagonal in the Fock basis. This can be understood by inspecting Eqs. (1.42) and (1.43), and keeping in mind that a linear combination of $\hat{x}_j$'s and $\hat{p}_j$'s is a linear combination of a_j's and $a_j^{\dagger}$'s. The vector parameter $\mathbf{r}$ is then just the vector of expectation values of the canonical operators on the state ϱ_G, which could be determined by performing measurements of positions and momenta on non-relativistic particles described by such operators. This will also be referred to as the vector of first (statistical) moments.

Let us then move on to consider second statistical moments of canonical operators on our state. In particular, let us consider the second moments in their symmetrised version, which we shall group together in the 'covariance matrix' $\boldsymbol{\sigma}$ (below, we will understand the anti-commutator between vectors to form a matrix, per the outer product compact notation introduced to express

the canonical commutation relations at the beginning of the chapter):

$$\begin{aligned}
\boldsymbol{\sigma} &= \mathrm{Tr}\left[\left\{(\hat{\mathbf{r}}-\mathbf{r}),(\hat{\mathbf{r}}-\mathbf{r})^{\mathsf{T}}\right\}\varrho_G\right] \\
&= \prod_{j=1}^{n}\left(1-\mathrm{e}^{-\xi_j}\right)\mathrm{Tr}\left[\left(\bigotimes_{j=1}^{n}\left(\sum_{m=0}^{\infty}\mathrm{e}^{-\xi_j m}|m\rangle_{jj}\langle m|\right)\right)\hat{S}\hat{D}_{\mathbf{r}}\left\{(\hat{\mathbf{r}}-\mathbf{r}),(\hat{\mathbf{r}}-\mathbf{r})^{\mathsf{T}}\right\}\hat{D}_{\mathbf{r}}^{\dagger}\hat{S}^{\dagger}\right] \\
&= \prod_{j=1}^{n}\left(1-\mathrm{e}^{-\xi_j}\right)\mathrm{Tr}\left[\left(\bigotimes_{j=1}^{n}\left(\sum_{m=0}^{\infty}\mathrm{e}^{-\xi_j m}|m\rangle_{jj}\langle m|\right)\right)\hat{S}\left\{\hat{\mathbf{r}},\hat{\mathbf{r}}^{\mathsf{T}}\right\}\hat{S}^{\dagger}\right] \\
&= \prod_{j=1}^{n}\left(1-\mathrm{e}^{-\xi_j}\right)\mathrm{Tr}\left[\left(\bigotimes_{j=1}^{n}\left(\sum_{m=0}^{\infty}\mathrm{e}^{-\xi_j m}|m\rangle_{jj}\langle m|\right)\right)\left\{S\hat{\mathbf{r}},\hat{\mathbf{r}}^{\mathsf{T}}S^{\mathsf{T}}\right\}\right] \\
&= \prod_{j=1}^{n}\left(1-\mathrm{e}^{-\xi_j}\right)S\mathrm{Tr}\left[\left(\bigotimes_{j=1}^{n}\left(\sum_{m=0}^{\infty}\mathrm{e}^{-\xi_j m}|m\rangle_{jj}\langle m|\right)\right)\left\{\hat{\mathbf{r}},\hat{\mathbf{r}}^{\mathsf{T}}\right\}\right]S^{\mathsf{T}}\ . \qquad (1.52)
\end{aligned}$$

Thanks to the use we made of group representations, we were able to bring the unitary operators outside the evaluation of the expectation value, which is now reduced to determining the trace in the last expression above. That is a rather straightforward task. First of all, notice that any expectation value involving two canonical operators pertaining to different modes is zero, because the state left inside the trace is diagonal in the Fock basis (this is the same argument by which we showed that the expectation values of linear functions of canonical operators are zero for such states). We are left with the task of evaluating the expectation values of the operators

$$2\hat{x}_j^2 = 2a_j^{\dagger}a_j + 1 + a_j^2 + a_j^{\dagger 2}\ , \qquad (1.53)$$

$$2\hat{p}_j^2 = 2a_j^{\dagger}a_j + 1 - a_j^2 - a_j^{\dagger 2}\ , \qquad (1.54)$$

$$\hat{x}_j\hat{p}_j + \hat{p}_j\hat{x}_j = i(a_j^{\dagger 2} - a_j^2)\ , \qquad (1.55)$$

which have been expressed as functions of creation and annihilation operators, for the local state $\sum_{m=0}^{\infty}\mathrm{e}^{-\xi_j m}|m\rangle_{jj}\langle m|$. Only terms with the same number of a_j and $a_j^{\dagger}$ contribute to the expectation value, because the state we are considering is diagonal in the Fock basis. The only operator that does contribute, besides the identity, is the number operator $a_j^{\dagger}a_j$, for which one finds

$$\langle a_j^{\dagger}a_j\rangle = \left(1-\mathrm{e}^{-\xi_j}\right)\mathrm{Tr}\left[\sum_{m=0}^{\infty}\mathrm{e}^{-\xi_j m}|m\rangle_{jj}\langle m|a_j^{\dagger}a_j\right] \qquad (1.56)$$

$$= \left(1-\mathrm{e}^{-\xi_j}\right)\sum_{m=0}^{\infty}\mathrm{e}^{-\xi_j m}m = \frac{\mathrm{e}^{-\xi_j}}{1-\mathrm{e}^{-\xi_j}}\ , \qquad (1.57)$$

so that

$$2\langle\hat{x}_j^2\rangle = 2\langle\hat{p}_j^2\rangle = \frac{2\mathrm{e}^{-\xi_j}}{1-\mathrm{e}^{-\xi_j}} + 1 = \frac{1+\mathrm{e}^{-\xi_j}}{1-\mathrm{e}^{-\xi_j}}\ . \qquad (1.58)$$

Hence, for the expectation values of the anti-commutators entering Eq. (1.52), one has

$$\prod_{j=1}^{n}\left(1-\mathrm{e}^{-\xi_j}\right)\mathrm{Tr}\left[\left(\bigotimes_{j=1}^{n}\left(\sum_{m=0}^{\infty}\mathrm{e}^{-\xi_j m}|m\rangle_{jj}\langle m|\right)\right)\left\{\hat{\mathbf{r}},\hat{\mathbf{r}}^{\mathsf{T}}\right\}\right]=\bigoplus_{j=1}^{n}\frac{1+\mathrm{e}^{-\xi_j}}{1-\mathrm{e}^{-\xi_j}}\mathbb{1}_2\ . \tag{1.59}$$

Upon defining

$$\nu_j=\frac{1+\mathrm{e}^{-\xi_j}}{1-\mathrm{e}^{-\xi_j}}\ , \tag{1.60}$$

the covariance matrix (CM) of the most general Gaussian state can be written as

$$\boldsymbol{\sigma}=S\left(\bigoplus_{j=1}^{n}\nu_j\mathbb{1}_2\right)S^{\mathsf{T}}\ , \tag{1.61}$$

with $\nu_j\geq 1$ [see Eq. (1.60)] and $S\in Sp_{2n,\mathbb{R}}$.

Eq. (1.61), formally analogous to (1.28), is the normal mode decomposition of the CM $\boldsymbol{\sigma}$, with ν_j as its symplectic eigenvalues.

The spectrum of the state ϱ_G is given in terms of the symplectic eigenvalues alone, as per

$$\varrho_G=\hat{D}_{\mathbf{r}}^{\dagger}\hat{S}^{\dagger}\left(\bigotimes_{j=1}^{n}\left(\sum_{m=0}^{\infty}2\left(\frac{\nu_j-1}{\nu_j+1}\right)^{m}|m\rangle_{jj}\langle m|\right)\right)\hat{S}\hat{D}_{\mathbf{r}}\ . \tag{1.62}$$

Eq. (1.61), along with (1.51), shows that all the parameters of a Gaussian state, $\mathbf{r}$, S and $\{\nu_j\}$, are completely determined by first and second statistical moments, which can then be adopted as a way to parametrise the state. This is in obvious analogy with a Gaussian distribution, which is also completely determined by first and second order moments. In the following, we will let covariance matrices represent Gaussian states, when first moments will be irrelevant, as is often the case.

1.6 The uncertainty principle

Not all symmetric matrices belong to the set of covariances of a quantum state. The non-commutativity of the canonical operators, along with the probabilistic interpretation of the quantum state, impose specific constraints on the variances and covariances of such observables that go under the name of uncertainty principles. We will derive here a geometric uncertainty relation which turns out to be necessary and sufficient for $\boldsymbol{\sigma}$ to be a the CM of a Gaussian state.

Given a – not necessarily Gaussian – quantum state ϱ on a system of n modes, let us define the matrix $\boldsymbol{\tau}$ as

$$\boldsymbol{\tau}=2\mathrm{Tr}\left[\varrho\hat{\mathbf{r}}\hat{\mathbf{r}}^{\mathsf{T}}\right]\ , \tag{1.63}$$

where $\hat{\mathbf{r}}\hat{\mathbf{r}}^{\mathsf{T}}$ is to be taken in the outer product sense. One has

$$\boldsymbol{\tau} = \mathrm{Tr}\left[\varrho\{\hat{\mathbf{r}}, \hat{\mathbf{r}}^{\mathsf{T}}\} + \varrho[\hat{\mathbf{r}}, \hat{\mathbf{r}}^{\mathsf{T}}]\right] = \boldsymbol{\sigma} + i\Omega\,. \tag{1.64}$$

Now, define the operator $\hat{O} = \sqrt{2}\,\mathbf{y}^{\dagger}\hat{\mathbf{r}}$ for a generic $\mathbf{y} \in \mathbb{C}^{2n}$. Because of the positivity of the density matrix ϱ, one has

$$0 \leq \mathrm{Tr}\left[\varrho\hat{O}\hat{O}^{\dagger}\right] = \mathbf{y}^{\dagger}\boldsymbol{\tau}\mathbf{y} = \mathbf{y}^{\dagger}(\boldsymbol{\sigma} + i\Omega)\mathbf{y}\,, \quad \forall\, \mathbf{y} \in \mathbb{C}^{2n}\,. \tag{1.65}$$

That is **(Robertson Schrödinger uncertainty relation)**

$$\boldsymbol{\sigma} + i\Omega \geq 0\,. \tag{1.66}$$

This relationship is manifestly invariant under symplectic transformations, since $\Omega = S\Omega S^{\mathsf{T}}$. It can therefore be expressed in terms of the symplectic eigenvalues, which are the n independent symplectic invariant quantities of a $2n$-mode covariance matrix. By writing (1.66) for the normal mode form of $\boldsymbol{\sigma}$ one gets

$$\boldsymbol{\nu} + i\Omega = \bigoplus_{j=1}^{n} \begin{pmatrix} \nu_j & 1 \\ -1 & \nu_j \end{pmatrix} \geq 0\,, \tag{1.67}$$

which is equivalent to

$$\nu_j \geq 1\,, \quad j \in [1, \ldots, n]\,. \tag{1.68}$$

It may be shown that (1.66) directly implies that $\boldsymbol{\sigma} > 0$, and hence that any $\boldsymbol{\sigma}$ pertaining to a quantum state can be symplectically diagonalised, so that (1.68) is completely equivalent to (1.66).

In our constructive definition of the set of Gaussian states, the relationship (1.68) arose naturally as a sufficient condition on the symplectic eigenvalues. Hence, we can claim that the uncertainty relation (1.66), which is equivalent to (1.68), is necessary and sufficient for $\boldsymbol{\sigma}$ to represent the covariance matrix of a Gaussian state.

1.7 Manipulation of Gaussian states

The tensor product of two Gaussian states is clearly still a Gaussian state, characterised as follows.

Tensor products of Gaussian states. By definition of $\mathbf{r}$ and $\boldsymbol{\sigma}$, one has that the global vector of first moments $\mathbf{r}$ and CM $\boldsymbol{\sigma}$ of the tensor product of two Gaussian states ϱ_A and ϱ_B, with first moments $\mathbf{r}_A$ and $\mathbf{r}_B$ and CMs $\boldsymbol{\sigma}_A$ and $\boldsymbol{\sigma}_B$, are given by

$$\mathbf{r} = \begin{pmatrix} \mathbf{r}_A \\ \mathbf{r}_B \end{pmatrix} = \mathbf{r}_A \oplus \mathbf{r}_B \ , \tag{1.69}$$

$$\boldsymbol{\sigma} = \begin{pmatrix} \boldsymbol{\sigma}_A & 0 \\ 0 & \boldsymbol{\sigma}_B \end{pmatrix} = \boldsymbol{\sigma}_A \oplus \boldsymbol{\sigma}_B \ . \tag{1.70}$$

Symplectic transformations on Gaussian states. In view of the above, a symplectic transformation S acts on the first moments $\mathbf{r}$ and second moments $\boldsymbol{\sigma}$ of a Gaussian state according to

$$\mathbf{r} \mapsto S\mathbf{r} \ , \tag{1.71}$$

$$\boldsymbol{\sigma} \mapsto S\boldsymbol{\sigma}S^{\mathsf{T}} \ . \tag{1.72}$$

Any symplectic transformation S can be decomposed into compact and non-compact symplectic transformations, as per

Singular value decomposition of symplectic transformations (aka "Euler" or "Bloch–Messiah" decomposition). Any symplectic matrix $S \in Sp_{2n,\mathbb{R}}$ can be decomposed as

$$S = O_1 Z O_2 \ , \tag{1.73}$$

with O_1, $O_2 \in Sp_{2n,\mathbb{R}} \cap SO(2n)$ and

$$Z = \bigoplus_{j=1}^{n} \begin{pmatrix} z_j & 0 \\ 0 & z_j^{-1} \end{pmatrix} \ . \tag{1.74}$$

The transformations O_1 and O_2, belonging to $SO(2n)$ (as well as $Sp_{2n,\mathbb{R}}$) preserve the identity, which represents the free Hamiltonian of the bosonic field. Hence, they are also referred to as "energy-preserving" or "passive" transformations. In turn, they can be decomposed into beam-splitters and phase-shifters, following the terminology in use in quantum optics.

More precisely, a beam splitter (a semi-reflectant mirror that mix two modes up) is described by an orthogonal on two modes mixing x's and p's in the same way:

$$S_{BS} = \begin{pmatrix} \cos\theta & 0 & \sin\theta & 0 \\ 0 & \cos\theta & 0 & \sin\theta \\ -\sin\theta & 0 & \cos\theta & 0 \\ 0 & -\sin\theta & 0 & \cos\theta \end{pmatrix} \ , \tag{1.75}$$

where $\cos^2\theta$ is the transmittivity of the semi-reflectant mirror, while a phase shifter (a dielectric plate that rotate the polarisation of a travelling electromagnetic wave with respect to a given reference) is simply a local rotation:

$$S_{PS} = \begin{pmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{pmatrix}, \tag{1.76}$$

where φ represents the phase shift of the polarisation vector.

Note that, if one switches to complex variables α, a phase shifter just multiplies α by a phase $\mathrm{e}^{i\varphi}$, while a beam splitter rotates α_1 and α_2. It may be shown that orthogonal symplectic transformations are isomorphic to unitary matrices in dimension n which, since any unitary can be decomposed into a product of diagonal local phase multiplication and 2×2 real rotations, allows one to prove that any passive symplectic operation is the product of beam splitter and phase shifters, given above.

Going back to the Euler decomposition, it is clear that it can be interpreted to state that any symplectic operation, and hence any purely quadratic operation at the Hilbert space level, can be decomposed as the product of passive operations and local squeezing operations, where by a local squeezing S_{SQ} we intend a symplectic acting on a single mode by contracting a canonical variable and expanding the conjugate one:

$$S_{SQ} = \begin{pmatrix} z_j & 0 \\ 0 & z_j^{-1} \end{pmatrix}. \tag{1.77}$$

In quantum optics, a squeezing operation is obtained by employing nonlinear crystals pumped by an accessory laser field, in set-ups which are referred to as parametric oscillators or parametric amplifiers (depending on whether the light field is in a cavity, or a travelling wave). Such operations require energy, in the sense that they do not commute with the free Hamiltonian.

Chapter 2

Phase Space methods

The language of statistical moments and covariance matrices we introduced in the previous chapter offers a compact and efficient formalism to deal with Gaussian states. A much more general approach may be taken to describe any quantum state in a setting which is reminiscent of classical phase space. This is the framework of characteristic functions and quasi-probability distributions, which goes back to seminal work by Wigner on quantum corrections to classical statistical mechanics, and bloomed in the sixties with the rise of theoretical quantum optics and the emergence of a general unifying picture.

Conceptually, the phase space description of quantum states hinges on the completeness of the set of displacement operators, which we shall prove in the form a Fourier-Weyl relation between density matrices and characteristic functions. This relationship will constitute the bridge between phase space and Hilbert space descriptions, which will be useful in several applications to quantum technologies. It will be convenient to handle most of the proofs and mathematical arguments concerning characteristic functions and quasi-probability distributions on a single mode of the system. Because displacement operators of multimode systems are just tensor products of local displacement operators, the extension of the formalism to systems with many degrees of freedom will be straightforward. Nevertheless, we shall always take care of explicitly linking the single-mode formulae which will appear in this chapter to the general multimode description adopted in the previous one.

2.1 Coherent states

The coherent state $|\alpha\rangle$ is the eigenvector of the operator a with eigenvalue α. If one defines $\alpha = \frac{x+ip}{\sqrt{2}}$, $\mathbf{r} = (x, p)^{\mathsf{T}}$ and the operator $\hat{D}_\alpha$ as

$$\hat{D}_\alpha = \hat{D}_{-\mathbf{r}} = \mathrm{e}^{-i\mathbf{r}^{\mathsf{T}}\Omega\hat{\mathbf{r}}} = \mathrm{e}^{\alpha a^\dagger - \alpha^* a}, \tag{2.1}$$

in keeping with the convention adopted in the previous chapter, one finds $\hat{D}_\alpha^\dagger a \hat{D}_\alpha = a + \alpha$.

The eigenstate $|\alpha\rangle$ is then easily determined as

$$\hat{D}_\alpha|0\rangle\,. \tag{2.2}$$

In fact, one has

$$a\hat{D}_\alpha|0\rangle = \hat{D}_\alpha\hat{D}_\alpha^\dagger a\hat{D}_\alpha|0\rangle = \hat{D}_\alpha(a+\alpha)|0\rangle = \alpha\hat{D}_\alpha|0\rangle\,. \tag{2.3}$$

The expression of $|\alpha\rangle$ in Fock basis is also readily established, and reads

$$|\alpha\rangle = \mathrm{e}^{-\frac{|\alpha|^2}{2}}\sum_{m=0}^{\infty}\frac{\alpha^m}{\sqrt{m!}}|m\rangle\,. \tag{2.4}$$

Two further relationships we will use throughout the chapter are the expression of the CCR for Weyl operators with complex variables

$$\hat{D}_\alpha\hat{D}_\beta = \mathrm{e}^{\frac{1}{2}(\alpha\beta^*-\alpha^*\beta)}\hat{D}_{\alpha+\beta} \tag{2.5}$$

and the overlap between two coherent states:

$$\begin{aligned}\langle\beta|\alpha\rangle &= \langle 0|\hat{D}_{-\beta}\hat{D}_\alpha|0\rangle = \langle 0|\hat{D}_{\alpha-\beta}|0\rangle\,\mathrm{e}^{\frac{1}{2}(\alpha\beta^*-\alpha^*\beta)}\\ &= \langle 0|\alpha-\beta\rangle\,\mathrm{e}^{\frac{1}{2}(\alpha\beta^*-\alpha^*\beta)} = \mathrm{e}^{-\frac{1}{2}|\alpha-\beta|^2}\,\mathrm{e}^{\frac{1}{2}(\alpha\beta^*-\alpha^*\beta)}\,.\end{aligned} \tag{2.6}$$

While not orthogonal, the coherent states form a complete set, in that the identity operator can be represented as a weighted integral of projectors on coherent states:

$$\frac{1}{\pi}\int_{\mathbb{C}}|\alpha\rangle\langle\alpha|\,\mathrm{d}^2\alpha = \mathbb{1}\,. \tag{2.7}$$

This can be seen by using the Fock basis decomposition (2.4):

$$\begin{aligned}\frac{1}{\pi}\int_{\mathbb{C}}\mathrm{d}^2\alpha\,|\alpha\rangle\langle\alpha| &= \frac{1}{\pi}\sum_{m,n=0}^{\infty}\int_{\mathbb{C}}\mathrm{d}^2\alpha\,\frac{\alpha^m\alpha^{*n}}{\sqrt{m!n!}}\,\mathrm{e}^{-|\alpha|^2}|m\rangle\langle n|\\ &= \frac{1}{\pi}\sum_{m,n=0}^{\infty}\int_0^\infty\mathrm{d}\rho\int_0^{2\pi}\mathrm{d}\varphi\,\mathrm{e}^{i(m-n)\varphi}\,\frac{\mathrm{e}^{-\rho^2}\rho^{m+n+1}}{\sqrt{m!n!}}|m\rangle\langle n|\\ &= \sum_m^\infty 2\int_0^\infty\mathrm{d}\rho\,\frac{\mathrm{e}^{-\rho^2}\rho^{2m+1}}{m!}|m\rangle\langle m| = \sum_{m=0}^{\infty}|m\rangle\langle m| = \mathbb{1}\,,\end{aligned} \tag{2.8}$$

where we used $\int_0^{2\pi}\mathrm{e}^{i(m-n)\varphi}\,\mathrm{d}\varphi = 2\pi\delta_{mn}$ and $\int_0^\infty\mathrm{e}^{-\rho^2}\rho^{2m+1}\,\mathrm{d}\rho = \frac{m!}{2}$.

Since they are not orthogonal and yet they resolve the identity as an integral of one-dimensional projectors, the coherent states form actually an *overcomplete* set, that is a set which is still complete after removal of any one element.

Eq. (2.8) implies that the trace of any trace-class operator $\hat{O}$ can be determined as an integral over coherent states:

$$\begin{aligned}\mathrm{Tr}\left[\hat{O}\right] &= \sum_{m=0}^{\infty}\langle m|\hat{O}|m\rangle = \frac{1}{\pi}\int_{\mathbb{C}}\mathrm{d}^2\alpha\sum_{m=0}^{\infty}\langle m|\alpha\rangle\langle\alpha|\hat{O}|m\rangle \\ &= \frac{1}{\pi}\int_{\mathbb{C}}\mathrm{d}^2\alpha\sum_{m=0}^{\infty}\langle\alpha|\hat{O}|m\rangle\langle m|\alpha\rangle = \frac{1}{\pi}\int_{\mathbb{C}}\mathrm{d}^2\alpha\,\langle\alpha|\hat{O}|\alpha\rangle\,. \end{aligned} \tag{2.9}$$

In terms of the language we developed in the previous chapter, it is immediately clear from the definition (2.2) that a coherent state $|\alpha\rangle$ is a Gaussian state with covariance matrix $\boldsymbol{\sigma} = \mathbb{1}$ and first moments $x = \mathrm{Re}(\alpha)/\sqrt{2}$ and $p = \mathrm{Im}(\alpha)/\sqrt{2}$ (recall that $\hat{D}_\alpha = \hat{D}^\dagger_{\mathbf{r}}$ with the definitions above for x and p).

2.2 A Fourier Weyl relation

We shall now establish a direct connection between density matrices on $L^2(\mathbb{R}^n)$ and functions of $2n$ variables, which stems from the fact that the displacement operators $\hat{D}_{\mathbf{r}}$ form an orthogonal complete set on the space of operators on $L^2(\mathbb{R}^n)$ with respect to the Hilbert–Schmidt scalar product. To this aim, we shall essentially follow the classical treatment due to Glauber. For simplicity, we will prove the statement explicitly for a single mode, adopting the complex single-mode notation $\hat{D}_\gamma$ for the Weyl operators. As anticipated above, the extension of such a result to the multimode case is straightforward.

Fourier-Weyl relation. Given bounded operator $\hat{O}$ on the Hilbert space of one bosonic mode, one has

$$\hat{O} = \frac{1}{\pi}\int_{\mathbb{C}}\mathrm{d}^2\alpha\,\mathrm{Tr}\left[\hat{D}_\alpha\hat{O}\right]\hat{D}_{-\alpha}\,. \tag{2.10}$$

Proof. First note that, due to the decomposition of the identity (2.8), any bounded operator $\hat{O}$ for which $\langle\alpha|\hat{O}|\beta\rangle$ is well defined may be decomposed as follows in terms of coherent states:

$$\hat{O} = \frac{1}{\pi^2}\int_{\mathbb{C}^2}\mathrm{d}\alpha\,\mathrm{d}\beta\,\langle\alpha|\hat{O}|\beta\rangle\,|\alpha\rangle\langle\beta|\,, \tag{2.11}$$

so that one just needs to prove that the operator $|\alpha\rangle\langle\beta|$ can be expanded in terms of displacement operators to extend the proof to all bounded operators. We intend to show that

$$|\alpha\rangle\langle\beta| = \frac{1}{\pi}\int_{\mathbb{C}}\mathrm{d}^2\gamma\,\mathrm{Tr}\left[|\alpha\rangle\langle\beta|\hat{D}_\gamma\right]\hat{D}^\dagger_\gamma\,. \tag{2.12}$$

Eq. (2.12) is equivalent to

$$\begin{aligned}
|0\rangle\langle 0| &= \frac{1}{\pi}\int_{\mathbb{C}} \mathrm{d}^2\gamma\, \mathrm{Tr}\left[|\alpha\rangle\langle\beta|\hat{D}_\gamma\right]\hat{D}_{-\alpha}\hat{D}_{-\gamma}\hat{D}_\beta \\
&= \frac{1}{\pi}\int_{\mathbb{C}} \mathrm{d}^2\gamma\, \mathrm{Tr}\left[|\alpha\rangle\langle\beta-\gamma|\right]\mathrm{e}^{\frac{1}{2}(\gamma\beta^*-\gamma^*\beta)}\hat{D}_{-\alpha}\hat{D}_{-\gamma}\hat{D}_\beta \\
&= \frac{1}{\pi}\int_{\mathbb{C}} \mathrm{d}^2\gamma\, \langle\beta-\gamma|\alpha\rangle\mathrm{e}^{\frac{1}{2}(\gamma\beta^*-\gamma^*\beta)}\hat{D}_{-\alpha}\hat{D}_{-\gamma}\hat{D}_\beta \\
&= \frac{1}{\pi}\int_{\mathbb{C}} \mathrm{d}^2\gamma\, \mathrm{e}^{-\frac{1}{2}|\beta-\alpha-\gamma|^2}\hat{D}_{\beta-\alpha-\gamma} = \frac{1}{\pi}\int_{\mathbb{C}} \mathrm{d}^2\gamma\, \mathrm{e}^{-\frac{1}{2}|\gamma|^2}\hat{D}_\gamma\ ,
\end{aligned}$$

where we used Eqs. (2.5) and (2.6). We are thus left with having to prove the following relationship:

$$|0\rangle\langle 0| = \frac{1}{\pi}\int_{\mathbb{C}} \mathrm{d}^2\gamma\, \mathrm{e}^{-\frac{1}{2}|\gamma|^2}\hat{D}_\gamma\ . \tag{2.13}$$

In order to do that, let us apply the operator on the right hand side on the Fock basis vector $|m\rangle$:

$$\begin{aligned}
\frac{1}{\pi}\int_{\mathbb{C}} \mathrm{d}^2\gamma\, \mathrm{e}^{-\frac{1}{2}|\gamma|^2}\hat{D}_\gamma\,|m\rangle &= \frac{1}{\pi}\int_{\mathbb{C}} \mathrm{d}^2\gamma\, \mathrm{e}^{-\frac{1}{2}|\gamma|^2}\hat{D}_\gamma\frac{a^{\dagger m}}{\sqrt{m!}}\,|0\rangle \\
&= \frac{1}{\pi}\int_{\mathbb{C}} \mathrm{d}^2\gamma\, \mathrm{e}^{-\frac{1}{2}|\gamma|^2}\frac{(a^\dagger-\gamma^*)^m}{\sqrt{m!}}\,|\gamma\rangle \\
&= \frac{1}{\pi}\int_{\mathbb{C}} \mathrm{d}^2\gamma \sum_{n=0}^{\infty} \mathrm{e}^{-|\gamma|^2}\frac{(a^\dagger-\gamma^*)^m}{\sqrt{m!}}\frac{\gamma^n}{\sqrt{n!}}\,|n\rangle \\
&= \sum_{n=0}^{\infty}\sum_{j=0}^{m}\frac{1}{\pi}\int_{\mathbb{C}} \mathrm{d}^2\gamma\, \mathrm{e}^{-|\gamma|^2}\binom{m}{j}(-1)^j\frac{\gamma^{*j}\gamma^n}{\sqrt{m!n!}}a^{\dagger(m-j)}\,|n\rangle \\
&= \sum_{j=0}^{m}\binom{m}{j}(-1)^j|m\rangle = \delta_{m0}|0\rangle\ ,
\end{aligned} \tag{2.14}$$

where we inserted the following integral, already employed in (2.8):

$$\frac{1}{\pi}\int_{\mathbb{C}} \mathrm{d}^2\gamma\, \mathrm{e}^{-|\gamma|^2}\gamma^{*j}\gamma^n = n!\,\delta_{jn}\ . \tag{2.15}$$

Eq. (2.14) is equivalent to (2.13) and hence to (2.12).

Characteristic function Given a state ϱ, we are thus led to define $\chi(\alpha) = \mathrm{Tr}[\hat{D}_\alpha\varrho]$ such that

$$\varrho = \frac{1}{\pi}\int_{\mathbb{C}} \mathrm{d}^2\alpha\,\chi(\alpha)\hat{D}_{-\alpha}\ . \tag{2.16}$$

As we will see in the next section, the function $\chi(\alpha)$ is known as the symmetrically ordered characteristic function associated to the quantum state ϱ. Clearly, complete knowledge of $\chi(\alpha)$ provides one with complete information about ϱ.

For a system of n modes, in the notation of the previous chapter, the Fourier Weyl relation we just derived reads

$$\varrho = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^{2n}} \mathrm{d}^{2n} r \, \chi(\mathbf{r}) \hat{D}_{\mathbf{r}} \, , \tag{2.17}$$

with $\mathrm{d}^{2n} r = \mathrm{d}x_1 \mathrm{d}p_1 \ldots \mathrm{d}x_n \mathrm{d}p_n$ and

$$\chi(\mathbf{r}) = \mathrm{Tr} \left[\hat{D}_{-\mathbf{r}} \varrho \right] \, . \tag{2.18}$$

Notice the change of sign due to the convention in defining $\hat{D}_\alpha$ set by Eq. (2.1). The additional factor $(1/2)^n$ is due to the change of measure associated with the change of variables $\alpha = \frac{x+ip}{\sqrt{2}}$.

Note also the orthogonality of the Weyl operators with respect to the Hilbert Schmidt norm:

$$\mathrm{Tr} \left[\hat{D}_\alpha \hat{D}_{-\beta} \right] = \pi \delta(\alpha - \beta) \, , \tag{2.19}$$

or, with $2n$ real variables,

$$\mathrm{Tr} \left[\hat{D}_{\mathbf{r}} \hat{D}_{-\mathbf{s}} \right] = (2\pi)^n \delta^{2n}(\mathbf{r} - \mathbf{s}) \, . \tag{2.20}$$

2.3 Characteristic functions and quasi-probability distributions

Given a quantum state ϱ of a single mode, the corresponding s-ordered characteristic function $\chi_s(\alpha)$ may be defined as

$$\chi_s(\alpha) = \mathrm{Tr} \left[\hat{D}_\alpha \varrho \right] \mathrm{e}^{\frac{s}{2}|\alpha|^2} \tag{2.21}$$

The significance of the exponential factor becomes manifest if one considers the evaluation of expectation values of ordered products of ladder operators. By recalling that $\hat{D}_\alpha = \mathrm{e}^{\alpha a^\dagger} \mathrm{e}^{-\alpha^* a} \mathrm{e}^{-\frac{1}{2}|\alpha|^2} = \mathrm{e}^{-\alpha^* a} \mathrm{e}^{\alpha a^\dagger} \mathrm{e}^{+\frac{1}{2}|\alpha|^2}$ and inserting such expressions in the definition of the s-ordered characteristic function, one obtains

$$\langle a^{\dagger m} a^n \rangle_1 = \mathrm{Tr} \left[a^{\dagger m} a^n \varrho \right] = \left(\frac{\partial}{\partial \alpha} \right)^m \left(-\frac{\partial}{\partial \alpha^*} \right)^n \chi_1(\alpha) \Big|_{\alpha=0} \, , \tag{2.22}$$

$$\langle a^{\dagger m} a^n \rangle_0 = \left(\frac{\partial}{\partial \alpha} \right)^m \left(-\frac{\partial}{\partial \alpha^*} \right)^n \chi_0(\alpha) \Big|_{\alpha=0} \, , \tag{2.23}$$

$$\langle a^{\dagger m} a^n \rangle_{-1} = \mathrm{Tr} \left[a^n a^{\dagger m} \varrho \right] = \left(\frac{\partial}{\partial \alpha} \right)^m \left(-\frac{\partial}{\partial \alpha^*} \right)^n \chi_{-1}(\alpha) \Big|_{\alpha=0} \, . \tag{2.24}$$

Differentiating the s-ordered characteristic function in $\alpha = 0$ allows one to retrieve the expectation value of s-ordered products of creation and annihilation

operators, with $s = 1$, $s = 0$ and $s = -1$ corresponding to normal, symmetric and anti-normal ordering respectively.[1]

Notice that the following relationship holds for all values of p:

$$\chi_s(0) = \mathrm{Tr}\,[\varrho] = 1\ . \tag{2.25}$$

By taking the complex Fourier transform of $\chi_s(\alpha)$ one may define the s-ordered "quasi-probability" distribution $W_s(\alpha)$:

$$W_s(\alpha) = \frac{1}{\pi^2}\int_{\mathbb{C}} \mathrm{d}^2\beta\, \mathrm{e}^{(\alpha\beta^* - \alpha^*\beta)}\chi_s(\beta)\ , \tag{2.26}$$

which is normalised:

$$\int_{\mathbb{C}} \mathrm{d}^2\alpha\, W_s(\alpha) = \chi_s(0) = 1 \tag{2.27}$$

and has the property that

$$\begin{aligned}\int_{\mathbb{C}} \mathrm{d}^2\alpha\, \alpha^{*m}\alpha^n W_s(\alpha) &= \frac{1}{\pi^2}\int_{\mathbb{C}} \mathrm{d}^2\alpha \int_{\mathbb{C}} \mathrm{d}^2\beta \left(\left(-\frac{\partial}{\partial\beta}\right)^m \left(\frac{\partial}{\partial\beta^*}\right)^n \mathrm{e}^{(\alpha\beta^* - \alpha^*\beta)}\right)\chi_s(\beta) \\ &= \int_{\mathbb{C}} \mathrm{d}^2\beta \left(\left(-\frac{\partial}{\partial\beta}\right)^m \left(\frac{\partial}{\partial\beta^*}\right)^n \delta(\beta)\right)\chi_s(\beta) \\ &= \left(\frac{\partial}{\partial\beta}\right)^m \left(-\frac{\partial}{\partial\beta^*}\right)^n \chi_s(\beta)\Big|_{\beta=0} = \langle a^{\dagger m} a^n\rangle_s\ ,\end{aligned} \tag{2.28}$$

where we applied the representation of the derivative of the delta function given by the integral over α. Eqs. (2.27) and (2.28) justify the terminology 'quasi-probability' distributions, with the "quasi-" there to remind one that the quantity $W_s(\alpha)$ is in general not positive, and in fact it may not even be a proper function at all, as we shall see in what follows.

Although they allow for a simple, unified treatment, the quasi-probability distributions for different values of s emerged historically at different times in different contexts, responding to different demands.

For $s = 1$, the quantity $W_1(\alpha)$ is the celebrated Glauber-Sudarshan P-representation, and is commonly denoted with $P(\alpha)$. One has the remarkable property:

Glauber-Sudarshan P-representation of a quantum state:

$$\varrho = \int_{\mathbb{C}} \mathrm{d}^2\alpha\, P(\alpha)|\alpha\rangle\langle\alpha|\ , \tag{2.29}$$

[1] In Eq. (2.23), we have implicitly defined the symmetric ordering of a product of $a^{\dagger m}$ and a^n as the normalised sum of products of m $a^\dagger$ and n a in all possible orders. For instance,

$$\langle a^{\dagger 2} a\rangle_0 = \mathrm{Tr}\left[\frac{1}{3}(a^{\dagger 2}a + a^\dagger a a^\dagger + a a^{\dagger^2})\varrho\right]\ .$$

which may be easily proven by applying the operator $\hat{D}_\alpha$ by similarity on both sides of Eq. (2.13), getting

$$|\alpha\rangle\langle\alpha| = \frac{1}{\pi}\int_{\mathbb{C}} \mathrm{d}^2\gamma\, \mathrm{e}^{-\frac{1}{2}|\gamma|^2}\mathrm{e}^{(\alpha\gamma^*-\alpha^*\gamma)}\hat{D}_{-\gamma}\ , \tag{2.30}$$

and then by inserting this expression in the right hand side of Eq. (2.29), to obtain

$$\begin{aligned}\int_{\mathbb{C}} \mathrm{d}^2\alpha\, P(\alpha)|\alpha\rangle\langle\alpha| &= \frac{1}{\pi}\int_{\mathbb{C}} \mathrm{d}^2\alpha \int_{\mathbb{C}} \mathrm{d}^2\gamma\, P(\alpha)\mathrm{e}^{-\frac{1}{2}|\gamma|^2}\mathrm{e}^{(\alpha\gamma^*-\alpha^*\gamma)}\hat{D}_{-\gamma} \\ &= \frac{1}{\pi}\int_{\mathbb{C}} \mathrm{d}^2\gamma\, \chi_1(\gamma)\mathrm{e}^{-\frac{1}{2}|\gamma|^2}\hat{D}_{-\gamma} = \frac{1}{\pi}\int_{\mathbb{C}} \mathrm{d}^2\gamma\, \chi_0(\gamma)\hat{D}_{-\gamma} = \varrho\ ,\end{aligned} \tag{2.31}$$

where we solved the integral over α through the inverse Fourier transform relation

$$\chi_1(\gamma) = \int_{\mathbb{C}} \mathrm{d}^2\alpha \mathrm{e}^{(\alpha\gamma^*-\alpha^*\gamma)}P(\alpha)\ , \tag{2.32}$$

and applied the Fourier-Weyl relation (2.12) in the last identity.

Due to their over-completeness, coherent states allow for a diagonal decomposition of any density matrix. However, this decomposition is given in terms of the quasi-probability $P(\alpha) = W_1(\alpha)$, which may be a distribution but not a proper function. For instance, the P-representation of a coherent state $|\alpha\rangle\langle\alpha|$ is the delta function $\delta(\gamma-\alpha)$, while the P-representation of a number state may only be expressed in term of derivatives of the delta function.

States with a P-representation "not more singular" than a delta function, including coherent states, are often referred to as 'classical' states. Within the subset of Gaussian states, it is easy to see that such states are those for which the smallest eigenvalue of the covariance matrix $\boldsymbol{\sigma}$ is greater than or equal to 1. We shall not discuss this notion further but we will employ it later on for a remarkable consequence it has when studying the separability of Gaussian states.

The Fourier-Weyl relation allows one to shed light on the nature of the anti-symmetrically ordered quasi-probability function $W_{-1}(\alpha)$ too. Such a function is commonly referred to as the 'Husimi' Q-function, and denoted as $Q(\alpha)$. One has

$$\begin{aligned}\frac{1}{\pi}\langle\alpha|\varrho|\alpha\rangle &= \frac{1}{\pi^2}\int_{\mathbb{C}} \mathrm{d}^2\beta\, \chi_0(\beta)\langle\alpha|\hat{D}_{-\beta}|\alpha\rangle = \frac{1}{\pi^2}\int_{\mathbb{C}} \mathrm{d}^2\beta\, \mathrm{e}^{\frac{1}{2}(\alpha\beta^*-\alpha^*\beta)}\chi_0(\beta)\langle\alpha|\alpha-\beta\rangle \\ &= \frac{1}{\pi^2}\int_{\mathbb{C}} \mathrm{d}^2\beta\, \mathrm{e}^{\alpha\beta^*-\alpha^*\beta}\chi_0(\beta)\mathrm{e}^{-\frac{|\beta|^2}{2}} = W_{-1}(\alpha) = Q(\alpha)\ .\end{aligned} \tag{2.33}$$

The Q-function is therefore always positive and does not diverge. On account of these properties, it found wide application in the study of quantum dynamical systems, whenever a well defined probability distribution is desirable. The value of the Q-function at a point α represents the probability that the 'heterodyne' measurement of the system yields the outcome α (heterodyne measurements give complex outcomes).

As for the symmetrically ordered $W_0(\alpha)$, it was historically the first quasi-probability to be introduced, by Wigner, and goes under the name of Wigner function. We shall denote it as $W(\alpha)$, omitting the subscript. Likewise, χ will represent the symmetrically ordered characteristic function χ_0. It is instructive to express the integral (2.26), that defines the Wigner function, in terms of real variables through the identifications $\alpha = \frac{x+ip}{\sqrt{2}}$ and $\beta = \frac{x'+ip'}{\sqrt{2}}$, obtaining

$$\begin{aligned} W(x,p) &= \frac{1}{\pi^2}\int_{\mathbb{R}}\int_{\mathbb{R}} \frac{\mathrm{d}x'\,\mathrm{d}p'}{2}\,\mathrm{e}^{i(px'-xp')}\chi_0(x',p') \\ &= \frac{1}{2\pi^2}\int_{\mathbb{R}}\int_{\mathbb{R}} \mathrm{d}x'\,\mathrm{d}p'\,\mathrm{e}^{i(px'-xp')}\int_{\mathbb{R}}\mathrm{d}q\,\langle q|\hat{D}_{-\frac{\mathrm{r}'}{2}}\varrho\hat{D}_{-\frac{\mathrm{r}'}{2}}|q\rangle \\ &= \frac{1}{2\pi^2}\int_{\mathbb{R}^3}\mathrm{d}q\,\mathrm{d}x'\,\mathrm{d}p'\,\mathrm{e}^{ipx'}\mathrm{e}^{ip'(q-x)}\langle q-\frac{x'}{2}|\varrho|q+\frac{x'}{2}\rangle \qquad (2.34) \\ &= \frac{1}{\pi}\int_{\mathbb{R}}\mathrm{d}x'\,\mathrm{e}^{ipx'}\langle x-\frac{x'}{2}|\varrho|x+\frac{x'}{2}\rangle = \frac{2}{\pi}\int_{\mathbb{R}}\mathrm{d}x'\,\mathrm{e}^{i2px'}\langle x-x'|\varrho|x+x'\rangle\,, \end{aligned}$$

where we expressed the trace, as well as the final result, in terms of the improper quadrature eigenvalues $|q\rangle$, as per Eq. (1.15), and $\hat{D}_{-\frac{\mathrm{r}'}{2}} = \mathrm{e}^{-i\frac{x'}{2}\hat{p}}\mathrm{e}^{i\frac{p'}{2}\hat{p}}\mathrm{e}^{i\frac{p'x'}{8}} = \mathrm{e}^{i\frac{p'}{2}\hat{p}}\mathrm{e}^{-i\frac{x'}{2}\hat{p}}\mathrm{e}^{-i\frac{p'x'}{8}}$ (after ordering via Baker-Campbell-Hausdorff). We also applied the representation of the delta function as an integral of complex exponentials.

Operation interpretation of the Wigner function. Eq. (2.34) implies that

$$\frac{1}{2}\int_{-\infty}^{+\infty}\mathrm{d}p\,W(x,p) = \langle x|\varrho|x\rangle\,. \qquad (2.35)$$

Up to a factor $\frac{1}{2}$, the integral of the Wigner function over a certain phase space quadrature, gives the probability of measuring the conjugate quadrature. This statement is clearly phase invariant, in the specific sense that, if one defines the generalised canonical operators $\hat{x}_\theta = \cos\theta\,\hat{x} - \sin\theta\,\hat{p}$ and associated canonical variables x_θ, one has

$$\frac{1}{2}\int_{-\infty}^{+\infty}\mathrm{d}x_{\theta-\frac{\pi}{2}}\,W(x,p) = \langle x_\theta|\varrho|x_\theta\rangle\,, \qquad (2.36)$$

since $[\hat{x}_\theta, \hat{x}_{\theta-\frac{\pi}{2}}] = i$.

The marginal of the Wigner function along any phase space direction is hence, up to a factor $\frac{1}{2}$, a positive probability distribution which describes the statistics of quadrature measurements. Such measurements, corresponding to position or momentum measurements for a material particle in the cases $\theta = 0, -\frac{\pi}{2}$, is implemented thorugh 'homodyne' detection in quantum optics.

2.4 Homodyne detection

Homodyne detection. A homodyne detection scheme consists in the measurement of the quadrature operator $\hat{x}_\theta = \cos\theta\hat{x} - \sin\theta\hat{p}$, with outcome probabilities:

$$p(x_\theta) = \langle x_\theta|\varrho|x_\theta\rangle \ . \tag{2.37}$$

Let us first notice that the operator $\hat{x}_\theta$ takes the following form in terms of ladder operators

$$\hat{x}_\theta = \frac{\mathrm{e}^{-i\theta}a + \mathrm{e}^{i\theta}a^\dagger}{\sqrt{2}} \ . \tag{2.38}$$

Homodyne detection results from mixing the initial state of a single-mode ϱ with a strong coherent state $|\alpha\rangle$ (with $\alpha = |\alpha|\mathrm{e}^{i\theta}$ and $|\alpha| \gg 1$) at a balanced (50:50) beam-splitter (given by Eq. (1.75) for $\theta = \pi/4$), and by subtracting the detected intensities at the two outputs of the beam-splitter. If a is the annihilation operator of the system mode and b is the annihilation operator of the coherent state, the outputs are described, in the Heisenberg picture, by the modes

$$\frac{a+b}{\sqrt{2}} \quad \text{and} \quad \frac{a-b}{\sqrt{2}} \ . \tag{2.39}$$

Subtraction of the two intensities then corresponds to measuring the operator

$$\frac{1}{2}(a+b)^\dagger(a+b) - \frac{1}{2}(a-b)^\dagger(a-b) = a^\dagger b + ab^\dagger \ , \tag{2.40}$$

with outcome probabilities $p(x)$ which have to be evaluated on the initial state (since we described the evolution in the Heisenberg picture). If $|\alpha| \gg 1$, then the state $|\alpha\rangle$, besides being by definition an eigenstate of b, approximates an eigenstate of $b^\dagger$ too, as

$$b^\dagger|\alpha\rangle = b^\dagger\hat{D}_\alpha|0\rangle = \hat{D}_\alpha(b^\dagger + \alpha^*)|0\rangle = \alpha^*|\alpha\rangle + \hat{D}_\alpha|1\rangle \simeq \alpha^*|\alpha\rangle \quad \text{for} \quad |\alpha| \gg 1 \, . \tag{2.41}$$

Hence, the operator being measured approximates the desired quadrature:

$$a^\dagger b + ab^\dagger \simeq |\alpha|\sqrt{2}\,\frac{\mathrm{e}^{-i\theta}a + \mathrm{e}^{i\theta}a^\dagger}{\sqrt{2}} = |\alpha|\sqrt{2}\hat{x}_\theta \ . \tag{2.42}$$

By varying the phase of the optical phase of the strong coherent state $|\alpha\rangle$, all the quadratures $\hat{x}_\theta$ may be scanned by the same apparatus (the pre-factor $|\alpha|\sqrt{2}$ is irrelevant, as it may just be handled by rescaling the measurement results).

2.5 Characteristic function of a Gaussian state

In order to link the phase space approach back to the material we introduced in the previous chapter, let us now determine the (symmetrically ordered) characteristic function χ_G of the most general Gaussian state, which was parametrised

in Eq. (1.48) in terms of a covariance matrix $\boldsymbol{\sigma} = S\boldsymbol{\nu}S^{\mathsf{T}}$ (with normal form $\boldsymbol{\nu}$) and a vector of first moments which we will denote here with $\mathbf{r}'$. We will start off with the general case with any number of variables, as in Eq. (2.18), and then reduce it to a single-mode problem, for which we will adopt more convenient complex variables.

By inserting Eq. (1.48) into Eq. (2.18) one gets

$$\begin{aligned}\chi_G(\mathbf{r})) &= \left(\prod_{j=1}^{n}\left(1-\mathrm{e}^{-\xi_j}\right)\right)\mathrm{Tr}\left[\left(\bigotimes_{j=1}^{n}\left(\sum_{m=0}^{\infty}\mathrm{e}^{-\xi_j m}|m\rangle_{jj}\langle m|\right)\right)\hat{S}\hat{D}_{\mathbf{r}'}D_{\mathbf{r}}\hat{D}^{\dagger}_{\mathbf{r}'}\hat{S}^{\dagger}\right]\\ &= \left(\prod_{j=1}^{n}\left(1-\mathrm{e}^{-\xi_j}\right)\right)\mathrm{Tr}\left[\left(\bigotimes_{j=1}^{n}\left(\sum_{m=0}^{\infty}\mathrm{e}^{-\xi_j m}|m\rangle_{jj}\langle m|\right)\right)D_{S^{-1}\mathbf{r}}\right]\mathrm{e}^{i\mathbf{r}'^{\mathsf{T}}\Omega\mathbf{r}},\end{aligned} \tag{2.43}$$

where we applied Eq. (1.11) and the projective representation of the symplectic group through the indentity

$$\hat{S}\hat{D}_{\mathbf{r}}\hat{S}^{\dagger} = \mathrm{e}^{i\mathbf{r}^{\mathsf{T}}\Omega S\hat{\mathbf{r}}} = \mathrm{e}^{i\mathbf{r}^{\mathsf{T}}S^{\mathsf{T}-1}\Omega\hat{\mathbf{r}}} = \hat{D}_{S^{-1}\mathbf{r}}\,. \tag{2.44}$$

Since the displacement operators are tensor products of local operators, the problem of determining χ_G has been reduced to finding the characteristic function of the single mode operator $\sum_{m=0}^{\infty}\mathrm{e}^{-\xi_j m}|m\rangle\langle m|$, where $|m\rangle$ is a Fock state. In fact, the characteristic function of a tensor product of operators is the product of their individual characteristic functions, so that the characteristic function of the Gaussian state may be determined, up to normalisation, by taking the product of such single-mode characteristic functions, multiplying it by the phase factor we determined above, and applying the symplectic transformation S^{-1} on the variable $\mathbf{r}$.

It is more expedient to evaluate the single-mode characteristic function of $\sum_{m=0}^{\infty}\mathrm{e}^{-\xi_j m}|m\rangle\langle m|$ by switching temporarily to complex variables:

$$\begin{aligned}\mathrm{Tr}\left[\sum_{m=0}^{\infty}\mathrm{e}^{-\xi_j m}|m\rangle\langle m|\hat{D}_{\alpha}\right] &= \frac{1}{\pi}\int_{\mathbb{C}}\mathrm{d}^2\gamma\,\sum_{m=0}^{\infty}\mathrm{e}^{-\xi_j m}\langle\gamma|m\rangle\langle m|\hat{D}_{\alpha}|\gamma\rangle\\ &= \frac{1}{\pi}\int_{\mathbb{C}}\mathrm{d}^2\gamma\,\mathrm{e}^{-\frac{1}{2}(|\gamma|^2+|\alpha+\gamma|^2+\alpha^*\gamma-\alpha\gamma^*)}\sum_{m=0}^{\infty}\frac{\left(\gamma^*(\alpha+\gamma)\mathrm{e}^{-\xi_j}\right)^m}{m!}\\ &= \frac{\mathrm{e}^{-\frac{|\alpha|^2}{2}}}{\pi}\int_{\mathbb{C}}\mathrm{d}^2\gamma\,\mathrm{e}^{-|\gamma|^2\left(1-\mathrm{e}^{-\xi_j}\right)}\mathrm{e}^{\alpha\gamma^*\mathrm{e}^{-\xi_j}-\alpha^*\gamma}\,.\end{aligned} \tag{2.45}$$

The latter is a standard Gaussian integral, which can be reduced to a particularly simple form by setting $\gamma = (x+iy)/\sqrt{1-\mathrm{e}^{-\xi_j}}$, and yields

$$\mathrm{Tr}\left[\sum_{m=0}^{\infty}\mathrm{e}^{-\xi_j m}|m\rangle\langle m|\hat{D}_{\alpha}\right] = \frac{\mathrm{e}^{-\frac{|\alpha|^2}{2}\left(\frac{1+\mathrm{e}^{-\xi_j}}{1-\mathrm{e}^{-\xi_j}}\right)}}{1-\mathrm{e}^{-\xi_j}} = \frac{\mathrm{e}^{-\frac{|\alpha|^2}{2}\nu_j}}{1-\mathrm{e}^{-\xi_j}}\,, \tag{2.46}$$

where we have inserted the symplectic eigenvalue of the covariance matrix $\boldsymbol{\sigma}$ according to Eq. (1.60). Combining Eqs. (2.43) and (2.46) leads to the following expression for the characteristic function of a multimode Gaussian state, after the substitution $\alpha = (x_j + ip_j)/\sqrt{2}$ for each different j:

$$\begin{aligned}\chi_G(\mathbf{r}) &= \mathrm{e}^{-\frac{1}{4}\mathbf{r}^\mathsf{T} S^{-1\mathsf{T}}(\bigoplus_{j=1}^n \nu_j \mathbb{1}_2) S^{-1}\mathbf{r}} \mathrm{e}^{i\mathbf{r}^\mathsf{T}\Omega^\mathsf{T}\mathbf{r}'} = \mathrm{e}^{-\frac{1}{4}\mathbf{r}^\mathsf{T} S^{-1\mathsf{T}}(\bigoplus_{j=1}^n \nu_j \mathbb{1}_2) S^{-1}\mathbf{r}} \mathrm{e}^{i\mathbf{r}^\mathsf{T}\Omega^\mathsf{T}\mathbf{r}'} \\ &= \mathrm{e}^{-\frac{1}{4}\mathbf{r}^\mathsf{T} S^{-1\mathsf{T}}\Omega^\mathsf{T}(\bigoplus_{j=1}^n \nu_j \mathbb{1}_2)\Omega S^{-1}\mathbf{r}} \mathrm{e}^{i\mathbf{r}^\mathsf{T}\Omega^\mathsf{T}\mathbf{r}'} = \mathrm{e}^{-\frac{1}{4}\mathbf{r}^\mathsf{T}\Omega^\mathsf{T} S(\bigoplus_{j=1}^n \nu_j \mathbb{1}_2) S^\mathsf{T}\Omega\mathbf{r}} \mathrm{e}^{i\mathbf{r}^\mathsf{T}\Omega^\mathsf{T}\mathbf{r}'} \\ &= \mathrm{e}^{-\frac{1}{4}\mathbf{r}^\mathsf{T}\Omega^\mathsf{T}\boldsymbol{\sigma}\Omega\mathbf{r}} \mathrm{e}^{i\mathbf{r}^\mathsf{T}\Omega^\mathsf{T}\mathbf{r}'} \,, \end{aligned} \tag{2.47}$$

where we exploited the invariance of $\left(\bigoplus_{j=1}^n \nu_j \mathbb{1}_2\right)$ under the action of Ω by congruence (the latter represents a product of local rotations on 2×2 subspaces, and thus preserves local identity matrices), and also repeatedly employed $S\Omega S^\mathsf{T} = \Omega$.

Characteristic function of a Gaussian state. Summarising, we have found that the characteristic function χ_G of a Gaussian state with covariance matrix $\boldsymbol{\sigma}$ and vector of first moments $\mathbf{r}'$ is given by:

$$\chi_G(\mathbf{r}) = \mathrm{e}^{-\frac{1}{4}\mathbf{r}^\mathsf{T}\Omega^\mathsf{T}\boldsymbol{\sigma}\Omega\mathbf{r}}\, \mathrm{e}^{i\mathbf{r}^\mathsf{T}\Omega^\mathsf{T}\mathbf{r}'} \,. \tag{2.48}$$

Notice how the vector variable $\mathbf{r}$ always enters this expression after multiplication by the symplectic form Ω.

We are thus led to yet another general characterisation of Gaussian states, as the quantum states with a Gaussian characteristic function. The Wigner function W_G of a Gaussian state, obtained by taking the complex Fourier transform of Eq. (2.48), is promptly evaluated, obtaining

$$\begin{aligned} W_G(\mathbf{r}) &= \frac{1}{2^n\pi^{2n}} \int_{\mathbb{R}^{2n}} \mathrm{d}^{2n}\mathbf{r}''\, \mathrm{e}^{-\frac{1}{4}\mathbf{r}''^\mathsf{T}\Omega^\mathsf{T}\boldsymbol{\sigma}\Omega\mathbf{r}''}\, \mathrm{e}^{i\mathbf{r}''^\mathsf{T}\Omega^\mathsf{T}(\mathbf{r}'-\mathbf{r})} \\ &= \frac{2^n}{\pi^n\sqrt{\mathrm{Det}\,\boldsymbol{\sigma}}}\, \mathrm{e}^{-(\mathbf{r}-\mathbf{r}')^\mathsf{T}\boldsymbol{\sigma}^{-1}(\mathbf{r}-\mathbf{r}')} \,. \end{aligned} \tag{2.49}$$

The latter is, with respect to the measure $\frac{\mathrm{d}^{2n}\mathbf{r}}{2^n}$, a Gaussian probability distribution centred in $\mathbf{r}'$ and with covariances described by $\boldsymbol{\sigma}$.

As we saw above, the marginal Wigner function along any phase space direction describes the probability distribution of the quantum measurement of the associated quadrature operator. Hence, as far as Gaussian states are concerned, the Wigner function provides one with a local, 'realistic' model to describe quadrature measurements. *If one restricts to quadrature measurements*, such systems may be mimicked by multivariate classical Gaussian distributions and will never show any signature of quantum non locality, such as a violation of Bell or CHSH inequalities. Clearly, quantum Gaussian states admit, besides the phase space description akin to classical distributions, an underlying Hilbert space description: general quantum measurements on the Hilbert space do allow for quantum non locality to become manifest with Gaussian states. It is however clear from the analogy with classical distributions that, whilst Gaussian

states are entirely described by first and second moments of their Wigner distributions, any analysis regarding genuinely quantum features, such as quantum entanglement, requires one to look beyond the phase space formalism.

Chapter 3

Entanglement of continuous variable systems

The characterisation of quantum correlations, also known as entanglement, is central to the study of quantum information. Entanglement turns out to be a key resource for the implementation of a number of quantum communication protocols, and also necessary to achieve computational speed-ups with quantum hardware, in the sense that accessing regions of the Hilbert space with entangled states allows one to shorten the computational depth of certain algorithms.

Not surprisingly, generating and maintaining entanglement is generally difficult in practice. Thanks to the techniques developed in quantum optical set-ups to achieve squeezed light, entanglement is however relatively straightforward to produce in optical quantum continuous variables. As we shall see, in fact, continuous variable entanglement is closely related to the notion of squeezing. It is therefore of the utmost importance to be able to qualify and quantify entanglement of continuous variables, which is the subject matter of the present chapter.

We will present criteria to detect the entanglement of Gaussian states and then proceed to describe a possible way to quantify such quantum correlations, bearing in mind that the determination of entanglement monotones of clear operational significance is still an open problem, even in the restricted arena of Gaussian states.

3.1 Entangled states and partial transposition

A bipartite quantum state ϱ_{AB} is said to be separable if and only if it can be written as a mixture of product states:

$$\varrho_{AB} = \sum_j p_j (\varrho_{A,j} \otimes \varrho_{B,j}) \, , \tag{3.1}$$

where $\varrho_{A,j}$ and $\varrho_{B,j}$ are local quantum states of subsystem A and B, respectively. Notice that the sum could generalise to an integral over continuous, real variables. A quantum state is entangled if and only if it is not separable.

A general sufficient criterion to detect entanglement, and one that, as we shall see, works very well with two-mode Gaussian states, is the so called positivity of the partial transposition (PPT) criterion: If ϱ_{AB} is separable, and so can be written as above, the partially transposed state $\varrho_{\tilde{AB}}$, *i.e.*, the state where transposition is applied to only one of the subsystems, say B to fix ideas, reads

$$\tilde{\varrho}_{AB} = \sum_j p_j (\varrho_{A,j} \otimes \varrho_{B,j}^{\mathsf{T}}) \tag{3.2}$$

and is still a quantum state. In particular, if ϱ_{AB} is separable, then $\tilde{\varrho}_{AB} \geq 0$ (the state is PPT). Therefore, if a state is such that $\varrho_{\tilde{AB}} \ngeq 0$, then it must be entangled (sufficient criterion for entanglement).

The PPT criterion is not necessary and sufficient as there exist entangled states, termed "bound-entangled" because they cannot be distilled, which are PPT. Note also that the transposition basis and subsystem are irrelevant to the positivity of the partially transposed state.

3.2 Separability criteria for Gaussian states

Let us dive straight into the action with a very general sufficient criterion for the separability of a Gaussian states:

Proposition. *An* (n)*-mode Gaussian state with CM* $\boldsymbol{\sigma} \geq 1$ *is separable across any bipartition of the modes.*

Proof. As we saw in chapter 2, a Gaussian state ϱ_G with CM $\boldsymbol{\sigma} \geq 1$ is classical, in the sense that its P-function $P(\mathbf{r})$ is not more singular than a delta function. Hence, such a state admits a P-representation as a convex sum of multimode coherent states:

$$\varrho_G = \int_{\mathbb{R}^n} \mathrm{d}^n \mathbf{r} P(\mathbf{r}) \hat{D}_{\mathbf{r}} |0\rangle\langle 0| \hat{D}_{\mathbf{r}}^\dagger \,. \tag{3.3}$$

Such a state is manifestly separable, as each $\hat{D}_{\mathbf{r}}|0\rangle$ is a product state since $\hat{D}_{\mathbf{r}}$ is always a tensor product of unitary operators on the two local Hilbert spaces. □

Besides providing an early hint as to the relationship between squeezing and entanglement[1], such a statement will serve as a powerful lemma in what follows to establish stricter criteria for separability.

[1] In that we just showed that the latter requires an eigenvalue of the covariance matrix smaller than 1, which in turn implies the existence of a canonical quadrature with noise lower than vacuum noise, *i.e.* "squeezing".

3.2.1 Separability of two-mode Gaussian states

The most basic, and arguably most relevant to experiments, separability problem in continuous variables concerns Gaussian states of 2 degrees of freedom. In this instance, an easily tested necessary and sufficient condition for separability can be derived, as we will see.

To lay the groundworks of our proof, let us introduce a decomposition of the CM $\boldsymbol{\sigma}$ of a 2-mode state into 2×2 sub-blocks, as per

$$\boldsymbol{\sigma} = \begin{pmatrix} \boldsymbol{\sigma}_A & \boldsymbol{\sigma}_{AB} \\ \boldsymbol{\sigma}_{AB}^{\mathsf{T}} & \boldsymbol{\sigma}_B \end{pmatrix} , \tag{3.4}$$

where $\boldsymbol{\sigma}_A$ and $\boldsymbol{\sigma}_B$ are the local CMs of the single-mode subsystems A and B, and $\boldsymbol{\sigma}_{AB}$ represents their correlations.

We can then move on to prove a reduction of a 2-mode CM $\boldsymbol{\sigma}$ to what is known as Simon's standard form:

Proposition. *Any two-mode covariance matrix $\boldsymbol{\sigma}$ may be reduced, by local, single-mode symplectic transformation into the standard form $\boldsymbol{\sigma}_{sf}$*

$$\boldsymbol{\sigma}_{sf} = \begin{pmatrix} a & 0 & c_+ & 0 \\ 0 & a & 0 & c_- \\ c_+ & 0 & b & 0 \\ 0 & c_- & 0 & b \end{pmatrix} \quad \text{with} \quad c_+ \geq c_- \ . \tag{3.5}$$

Proof. By Williamson theorem, local symplectic operations may be found to bring $\boldsymbol{\sigma}_A$ and $\boldsymbol{\sigma}_B$ into their normal mode form, $a\mathbb{1}_2$ and $b\mathbb{1}_2$ respectively. Such local submatrices are obviously invariant under local rotations, which are always symplectic. Through such rotations the off-diagonal block $\boldsymbol{\sigma}_{AB}$ may be diagonalised as per its singular value decomposition, which has also enough freedom to ensure $c_+ \geq c_-$. □

Notice that any quantity which may be affected by local unitary operations cannot play any role in determining the separability of a quantum state. Hence, as far Gaussian states are concerned, first moments, which can be arbitrarily adjusted by tensor products of local, unitary, displacement operators, can be safely disregarded. As for second moments of two-mode Gaussian states, only the locally invariant quantities entering Simon's standard form may have a bearing on the quantum correlations.

Simon's standard form may be adopted to obtain a more detailed condition for the separability of two-mode Gaussian states:

Proposition. *Two-mode Gaussian states with* $\mathrm{Det}\boldsymbol{\sigma}_{AB} \geq 0$ *are separable.*

Proof. Let us first take into account the case $\mathrm{Det}\boldsymbol{\sigma}_{AB} > 0$. As we just saw, the initial CM $\boldsymbol{\sigma}$ of any two-mode state can be turned by local unitary operations to the standard form $\boldsymbol{\sigma}_{sf}$ of Eq. (3.7), whose covariances may be arranged to have $a \geq b$ and $c_+ \geq c_- > 0$ without loss of generality. Let us then consider the

local symplectic transformation $S_{loc} = \mathrm{diag}(\sqrt{xy}, 1/\sqrt{xy}, \sqrt{y/x}, \sqrt{x/y})$, made up by the tensor product of local squeezings. With the choices

$$x = \sqrt{\frac{c_+ a + c_- b}{c_- a + c_+ b}}\,,$$

$$y = \sqrt{\frac{a/x + bx - [(a/x - bx)^2 + 4c_-^2]^{1/2}}{ax + b/x - [(ax - b/x)^2 + 4c_-^2]^{1/2}}}\,,$$

it can be directly shown that $\boldsymbol{\sigma}' = S_{loc}^{\mathsf{T}} \boldsymbol{\sigma}_{sf} S_{loc}$ may be diagonalized by a symplectic rotation R_{BS} of the form of Eq. (1.75), with a proper choice of the angle θ. *This would not be possible if c_+ and c_- had different signs.* Moreover, the smallest eigenvalue of this diagonal form is degenerate:

$$R_{12,\theta}^{\mathsf{T}} S_{loc}^{\mathsf{T}} \boldsymbol{\sigma}_{sf} S_{loc} R_{12,\theta} = \boldsymbol{\sigma}_{dg} = \mathrm{diag}\left(\kappa_1, \kappa_2, \kappa_-, \kappa_-\right),$$

with $\kappa_i \geq \kappa_-$ for $i = 1, 2$. But then, for such a diagonal CM, the uncertainty principle $\boldsymbol{\sigma}_{dg} + i\Omega \geq 0$ straightforwardly implies $\kappa_- \geq 1$. The Gaussian state with CM $\boldsymbol{\sigma}_{dg}$ is thus classical and therefore separable. So it is the Gaussian state with CM $\boldsymbol{\sigma}'$, related to $\boldsymbol{\sigma}_{dg}$ by a rotation, which cannot change the eigenvalues. The initial state, with CM $\boldsymbol{\sigma}$, is then separable as well, being related to the Gaussian state with CM $\boldsymbol{\sigma}'$ by local unitary operations. This completes the proof in the instance $\mathrm{Det}\boldsymbol{\sigma}_{AB} > 0$.

For $\mathrm{Det}\boldsymbol{\sigma}_{AB} = 0$, so that in $\boldsymbol{\sigma}_{sf}$ one has $c_+ \geq c_- = 0$, the proof is easier. In this instance a local squeezing $S_l = \mathrm{diag}\left(\sqrt{a}, 1/\sqrt{a}, \sqrt{b}, 1/\sqrt{b}\right)$ is needed to bring $\boldsymbol{\sigma}_{sf}$ into a form $\boldsymbol{\sigma}''$ with diagonal entries $\{a^2, 1, b^2, 1\}$ and only two nonzero off diagonal entries with value abc_+. The uncertainty principle $\boldsymbol{\sigma}'' + i\Omega \geq 0$ for a matrix $\boldsymbol{\sigma}''$ with such a form implies $\boldsymbol{\sigma}'' \geq \mathbb{1}$, thus establishing the separability of the original Gaussian state with CM $\boldsymbol{\sigma}$ and concludes our proof. □

Proposition. *The quantity $\Delta = \mathrm{Det}\boldsymbol{\sigma}_A + \mathrm{Det}\boldsymbol{\sigma}_B + 2\mathrm{Det}\boldsymbol{\sigma}_{AB}$ is invariant under symplectic transformations.*

Proof. Notice first that Δ is invariant under local symplectic transformations $S_A \otimes S_B$, because all such local transformations have determinant 1 and, acting by congruence, just multiply the 2×2 blocks without mixing them. Now, local operations may bring any initial $\boldsymbol{\sigma}$ in the standard form (3.7), with $\Delta = a^2 + b^2 + 2c_+c_-$. By reordering the variables (namely, by swapping the second and third one), any CM may be rewritten as

$$\boldsymbol{\sigma}' = \begin{pmatrix} \boldsymbol{\sigma}_x & \boldsymbol{\sigma}_{xp} \\ \boldsymbol{\sigma}_{xp}^{\mathsf{T}} & \boldsymbol{\sigma}_p \end{pmatrix}, \tag{3.6}$$

where $\boldsymbol{\sigma}_x$ pertains to the variables $\hat{x}_A$ and $\hat{x}_B$, $\boldsymbol{\sigma}_p$ pertains to $\hat{p}_A$ and $\hat{p}_B$, while $\boldsymbol{\sigma}_{xp}$ reports the $\hat{x} - \hat{p}$ correlations, with associated standard form

$$\boldsymbol{\sigma}'_{sf} = \begin{pmatrix} a & c_+ & 0 & 0 \\ c_+ & b & 0 & 0 \\ 0 & 0 & a & c_- \\ 0 & 0 & c_- & b \end{pmatrix} \quad \text{with} \quad c_+ \geq c_-\,. \tag{3.7}$$

Under such a different convention, the quantity Δ can be rewritten as

$$\Delta = a^2 + b^2 + 2c_+c_- = \mathrm{Tr}(\boldsymbol{\sigma}_x\boldsymbol{\sigma}_p) \; . \tag{3.8}$$

Notice also that the beam-splitting symplectic transformation of Eq. (1.75) corresponds, after reordering the variables, to two identical rotations acting on $\boldsymbol{\sigma}_x$ and $\boldsymbol{\sigma}_p$: such rotations do not affect Δ, as apparent from the expression (3.8). At the same time, such rotations, supplemented by local symplectic operations, are enough to bring $\boldsymbol{\sigma}'_{sf}$ into normal form: to this aim one may in fact rotate through a beam splitter to diagonalise, say, $\boldsymbol{\sigma}_p$, then apply a local squeezing transformation $S_{z_1,z_2} = \mathrm{diag}(z_1, z_2, 1/z_1, 1/z_2)$ to make $\boldsymbol{\sigma}_p$ invariant under rotations, and then apply a second beam splitter in order to diagonalise $\boldsymbol{\sigma}_x$ too. Local squeezing transformations are then sufficient to achieve normal form.

We have hence shown that one can bring any given two-mode CM $\boldsymbol{\sigma}$ to its normal form by symplectic transformations that do not affect Δ. The quantity Δ must then be completely determined by the symplectic eigenvalues ν_+ and ν_- of $\boldsymbol{\sigma}$ (with $\nu_+ \geq \nu_-$) as $\Delta = \nu_+^2 + \nu_-^2$ (this relation just follows from the definition of Δ applied to the normal form $\nu_+ \mathbb{1}_2 \oplus \nu_- \mathbb{1}_2$), and is hence a symplectic invariant itself. $\square$

Notice that another symplectic invariant quantity must exist, since there are as many independent symplectic invariants as the the number of symplectic eigenvalues, that is of the number of modes (two, in the present case). Such an invariant is simply $\mathrm{Det}(\boldsymbol{\sigma}) = \nu_+^2\nu_-^2$ which, by Binet theorem, is not affected by symplectic transformations S, whose determinant always equals 1. Note that, for a two-mode system, one has then:

$$\nu_\mp^2 = \frac{\Delta \mp \sqrt{\Delta^2 - 4\mathrm{Det}\boldsymbol{\sigma}}}{2} \; . \tag{3.9}$$

Let us now recall the reader that the positivity of a Gaussian state ϱ_G is equivalent to the condition $\boldsymbol{\sigma} + i\Omega \geq 0$ on its covariance matrix $\boldsymbol{\sigma}$, which can in turn be recast as $\nu_\mp \geq 1$ for the symplectic eigenvalues of a two-mode $\boldsymbol{\sigma}$ (see Section 1.6). It is easy to show that the positivity condition is completely equivalent to the following set of conditions on the CM $\boldsymbol{\sigma}$ of a two-mode state:

$$\mathrm{Det}\boldsymbol{\sigma} - \Delta + 1 \geq 0 \; , \tag{3.10}$$

$$\mathrm{Det}\boldsymbol{\sigma} \geq 1 \quad , \tag{3.11}$$

$$\boldsymbol{\sigma} > 0 \; . \tag{3.12}$$

The condition $\boldsymbol{\sigma} > 0$ must be specified because quadratic functions of the symplectic eigenvalues such as $\mathrm{Det}\boldsymbol{\sigma}$ and Δ will never be able to distinguish their sign. Also notice that $\boldsymbol{\sigma} > 0$, being sufficient for the existence of a normal form, implies that the symplectic eigenvalues as determined by (3.9) must be real, and thus subsumes $\Delta^2 \geq 4\mathrm{Det}\boldsymbol{\sigma}$: no positive matrix violating this inequality exists. The set of equations (3.10-3.12) form an explicit necessary and sufficient condition for a Gaussian operator, such as ϱ_G, to be positive. Such a characterisation of positivity will prove useful in the following.

We are now in a position to derive a necessary and sufficient criterion for the separability of two-mode Gaussian states. We already saw that the positivity of the partial transposition $\tilde{\varrho} \geq 0$ is a necessary condition for the separability of any quantum state ϱ, regardless of the Hilbert space dimension (and hence its violation is a sufficient condition for the entanglement). We are about to show that such criterion is also sufficient for the separability of two-mode Gaussian states. Before proving that, let us understand how partial transposition in the Hilbert space may be represented at the level of a phase space description. We are, in other words, interested in the effect of transposition on the canonical operators $\hat{x}$ and $\hat{p}$ of a single canonical degree of freedom. This can be determined by noticing that, in the Fock basis, the action of a and $a^\dagger$ can be written entirely with real coefficients and, therefore, one has $a^\mathsf{T} = a^\dagger$ and $a^{\dagger\mathsf{T}} = a$ (bear in mind that the positivity of the partial transposition is invariant under the choice of the transposition basis, which amounts to applying a certain local unitary to the quantum state). One is led to conclude:

$$\hat{x}^\mathsf{T} = \frac{(a + a^\dagger)^\mathsf{T}}{\sqrt{2}} = \hat{x} \, , \tag{3.13}$$

$$\hat{p}^\mathsf{T} = \frac{(a - a^\dagger)^\mathsf{T}}{i\sqrt{2}} = -\hat{p} \, . \tag{3.14}$$

Partial transposition can thus be represented, on the canonical operators of two degrees of freedom, by the action of the linear operator $T = \mathrm{diag}(1, 1, 1, -1)$, which mirror reflects one of the four variables. At the level of covariance matrices, this corresponds to the mapping $\boldsymbol{\sigma} \mapsto \tilde{\boldsymbol{\sigma}} = T\boldsymbol{\sigma}T$, where $\tilde{\boldsymbol{\sigma}}$ stands for the partially transposed CM.

PPT criterion for two-mode Gaussian states. The positivity of the partially transposed state is necessary and sufficient for the separability of a two-mode Gaussian state.

Proof. Consider a two-mode Gaussian state ϱ_G with CM $\boldsymbol{\sigma}$ decomposed according to Eq. (3.4) and satisfying the physicality conditions (3.10-3.12). The conditions (3.10-3.12) for the positivity of a Gaussian operator only depend on $\mathrm{Det}\boldsymbol{\sigma}$, Δ and the fact that $\boldsymbol{\sigma} > 0$. Partial transposition, acting on $\boldsymbol{\sigma}$ by congruence as per $\tilde{\boldsymbol{\sigma}} = T\boldsymbol{\sigma}T$ with $\mathrm{Det}T = 1$, cannot affect the determinant: $\mathrm{Det}\boldsymbol{\sigma} = \mathrm{Det}\tilde{\boldsymbol{\sigma}}$. Nor can it affect strict positivity: $\boldsymbol{\sigma} > 0$ implies $\tilde{\boldsymbol{\sigma}} > 0$. Then, the only relevant quantity affected by partial transposition must be $\Delta = \mathrm{Det}\boldsymbol{\sigma}_A + \mathrm{Det}\boldsymbol{\sigma}_B + 2\mathrm{Det}\boldsymbol{\sigma}_{AB}$, which turns into $\tilde{\Delta} = \mathrm{Det}\boldsymbol{\sigma}_A + \mathrm{Det}\boldsymbol{\sigma}_B - 2\mathrm{Det}\boldsymbol{\sigma}_{AB}$, because the effect of T is flipping the signs of both a column and a row, which leaves $\mathrm{Det}\boldsymbol{\sigma}_A$ and $\mathrm{Det}\boldsymbol{\sigma}_B$ alone but flips the sign of $\mathrm{Det}\boldsymbol{\sigma}_{AB}$. The expression of a necessary condition for separability in terms of second moments is hence

$$\mathrm{Det}\boldsymbol{\sigma} - \tilde{\Delta} + 1 \geq 0 \, . \tag{3.15}$$

One has then only to run through three possible instances, depending on the sign of $\mathrm{Det}\boldsymbol{\sigma}_{AB}$ and on whether (3.15) is satisfied or not.

If $\mathrm{Det}\boldsymbol{\sigma}_{AB} \geq 0$ then the state is separable according to a previous proposition, and (3.15) is necessarily satisfied since for $\mathrm{Det}\boldsymbol{\sigma}_{AB} \geq 0$, $\tilde{\Delta} \leq \Delta$ such that $\mathrm{Det}\boldsymbol{\sigma} - \tilde{\Delta} + 1 \geq \mathrm{Det}\boldsymbol{\sigma} - \Delta + 1 \geq 0$.

If $\mathrm{Det}\boldsymbol{\sigma}_{AB} < 0$ and (3.15) is not satisfied, then the state is entangled, because a violation of such a relationship is sufficient for the state to be entangled.

Finally, if $\mathrm{Det}\boldsymbol{\sigma}_{AB} < 0$ and (3.15) is satisfied, then the partially transposed state $\tilde{\varrho}_G$ is a Gaussian operator that satisfies all three conditions (3.10-3.12) and for which $\mathrm{Det}\tilde{\boldsymbol{\sigma}}_{AB} > 0$. That is, $\tilde{\varrho}_G$ is a separable physical quantum state. But then, the original state must be separable too, because partial transposition preserves separability.

The criterion (3.15) is hence necessary and sufficient for the separability of two-mode Gaussian states. □

3.3 Quantifying entanglement: Logarithmic negativity of Gaussian states

The logarithmic negativity is an entanglement monotone that, while not amenable to a clear operational interpretation, can often be evaluated exactly. This is the case for Gaussian states too, as we will show in the present section.

The logarithmic negativity $E_{\mathcal{N}}$ of a bipartite quantum state ϱ is defined, in terms of its partial transpose $\tilde{\varrho}$, as

$$E_{\mathcal{N}} = \log_2 \|\tilde{\varrho}\|_1 \,, \tag{3.16}$$

where $\|\hat{o}\|$ denotes the trace norm of operator $\hat{o}$, i.e. the sum of the absolute value of its eigenvalues of $\hat{o}$, if diagonalisable. Note that partial transposition cannot change the trace of an operator, so that the sum of the eigenvalues of a partially transposed state $\tilde{\varrho}$ is still 1. The quantity $\|\tilde{\varrho}\|_1$ may hence be different from – and in particular larger than – 1 if and only if $\tilde{\varrho}$ has negative eigenvalues. It follows that $E_{\mathcal{N}}$ is equal to 0 for all states with positive partial transpose, and larger than 1 for all states which violate the PPT criterion. The adoption of the logarithmic negativity is therefore somewhat unsatisfactory, in that there exist entangled states, known as "bound entangled" states, that have positive partial transpose, for which the logarithmic negativity is zero. Even so, the logarithmic negativity is still a consistent entanglement monotone – a quantity that does not increase under local operations and classical communication – and is related to entanglement distillation in the sense that it provides an upper bound to the asymptotic conversion rate between the state in question and entangled Bell pairs. The $\log_2$ occurring in Eq. (3.16) is needed for the logarithmic negativity to provide one with such an upper bound.

The quantity $\|\tilde{\varrho}_G\|_1 \mathrm{Tr}(|\tilde{\varrho_G}|)$ is promptly evaluated for Gaussian states of $m+n$ modes with CM $\boldsymbol{\sigma}$. Let $\tilde{\boldsymbol{\sigma}} = T\boldsymbol{\sigma}T$ be the partially transposed covariance matrix, where partial transposition with respect to the last n modes is described by $T = \bigoplus_{j=1}^{m} \mathbb{1}_2 \oplus \bigoplus_{j=1}^{n} \sigma_z$. Now, let $\{\tilde{\nu}_j, j \in [0, \ldots, m+n]\}$ be the symplectic eigenvalues of the partially transposed CM $\tilde{\boldsymbol{\sigma}}$. The constructive characterisation

of Gaussian states we went through in Chapter 1, allows us to cast the Gaussian operator $\tilde{\varrho_G}$ in the form

$$\tilde{\varrho}_G = \hat{D}_{\mathbf{r}}^{\dagger}\hat{S}^{\dagger}\left(\bigotimes_{j=1}^{n}\left(\sum_{m=0}^{\infty} 2\frac{(\tilde{\nu}_j-1)^m}{(\tilde{\nu}_j+1)^{m+1}}|m\rangle_{jj}\langle m|\right)\right)\hat{S}\hat{D}_{\mathbf{r}} \tag{3.17}$$

(where we just replaced ν_j in Eq. (1.62) with $\tilde{\nu}_j$) for some unitary operators $\hat{S}$ and $\hat{D}_{\mathbf{r}}$. As one should expect, only partially transposed normal modes with $\tilde{\nu}_j < 1$ contribute negative eigenvalues to the tensor product spectrum. The operator $|\tilde{\varrho_G}|$ is simply

$$|\tilde{\varrho}_G| = \hat{D}_{\mathbf{r}}^{\dagger}\hat{S}^{\dagger}\left(\bigotimes_{j=1}^{n}\left(\sum_{m=0}^{\infty} 2\frac{|\tilde{\nu}_j-1|^m}{(\tilde{\nu}_j+1)^{m+1}}|m\rangle_{jj}\langle m|\right)\right)\hat{S}\hat{D}_{\mathbf{r}}\ . \tag{3.18}$$

Clearly, the unitary operations $\hat{D}_{\mathbf{r}}$ and $\hat{S}$ do not affect the trace of $|\tilde{\varrho}_G|$. Also, the trace is multiplicative under tensor products ($\mathrm{Tr}(\varrho_A\otimes\varrho_B)=\mathrm{Tr}(\varrho_A)\mathrm{Tr}(\varrho_B)$ for trace class ϱ_A and ϱ_B), so that each term in the central tensor product contributes multiplicatively to $\mathrm{Tr}(|\tilde{\varrho}_G|)$. The factors with $\tilde{\nu}_j \geq 1$ are the same as those of a physical Gaussian state, and hence normalised. It will therefore suffice to consider the contribution of operators with $\tilde{\nu}_j < 1$, which are straightforwardly evaluated as geometric sums:

$$\frac{2}{\tilde{\nu}_j+1}\sum_{m=0}^{\infty}\left(\frac{1-\tilde{\nu}_j}{\tilde{\nu}_j+1}\right)^m = \frac{2}{\tilde{\nu}_j+1}\frac{\tilde{\nu}_j+1}{2\tilde{\nu}_j} = \frac{1}{\tilde{\nu}_j}\ . \tag{3.19}$$

Hence, one obtains

$$\|\tilde{\varrho}_G\|_1 = \prod_{j=1}^{m+n}\max\left\{1,\frac{1}{\tilde{\nu_j}}\right\} \tag{3.20}$$

and

$$E_{\mathcal{N}}\left(\varrho_G\right) = \sum_{j=1}^{m+n}\max\left\{0,-\log_2(\tilde{\nu}_j)\right\}\ . \tag{3.21}$$

The situation is particularly simple for two-mode systems, where it can be proven that, when partially transposing a physical state (*i.e.*, one with $\boldsymbol{\sigma}+i\Omega\geq 0$) with respect to one mode, only one of the two partially transposed symplectic eigenvalues can be smaller than 1. The two partially transposed eigenvalues are obtained by transposing the invariant Δ in Eq. (3.9):

$$\tilde{\nu}_{\mp}^2 = \frac{\tilde{\Delta}\mp\sqrt{\tilde{\Delta}^2-4\mathrm{Det}\boldsymbol{\sigma}}}{2}\ , \tag{3.22}$$

and the logarithmic negativity of a two-mode state $\varrho_{G,1+1}$ reads

$$E_{\mathcal{N}}(\varrho_{G,1+1}) = \max\left\{0,-\log_2\tilde{\nu}_-\right\}\ . \tag{3.23}$$

Logarithmic negativity of two-mode states. Summing up, the systematic recipe to verify and quantify the entanglement of a two-mode Gaussian state $\varrho_{G,1+1}$ with CM

$$\boldsymbol{\sigma} = \begin{pmatrix} \boldsymbol{\sigma}_A & \boldsymbol{\sigma}_{AB} \\ \boldsymbol{\sigma}_{AB}^{\mathsf{T}} & \boldsymbol{\sigma}_B \end{pmatrix} , \tag{3.24}$$

comprises the following steps:

1. Determine the two partially transposed symplectic invariants $\mathrm{Det}\boldsymbol{\sigma}$ and $\tilde{\Delta} = \mathrm{Det}\boldsymbol{\sigma}_A + \mathrm{Det}\boldsymbol{\sigma}_B - 2\mathrm{Det}\boldsymbol{\sigma}_{AB}$ (notice the minus sign that distinguishes $\tilde{\Delta}$ from Δ).

2. Determine $\tilde{\nu}_-$ according to Eq. (3.22) ($\tilde{\nu}_+$ is not needed). The state is entangled if and only if $\tilde{\nu}_- < 1$.

3. Determine the logarithmic negativity according to Eq. (3.23).

Chapter 4

Quantum estimation with Gaussian states

Imagine one has access to quantum means and wants to determine the value of an unknown real parameter, say ϑ, that characterises an operation Φ_ϑ, whose form is otherwise known. In practice, ϑ would typically be a temperature, or a parameter that characterises a Hamiltonian operator (such as an interaction time, or strength, or the product of the two). This is the vanilla version of the problem of 'parameter estimation' in quantum metrology. Occasionally, a variation of this issue when one attempts to establish whether a certain parameter is different from zero is referred to as 'quantum sensing'.

A very natural approach to determining ϑ is to prepare a certain quantum state ϱ, let it undergo the unknown operation Φ_ϑ, and finally measure the state through some POVM $\sum_\mu \hat{K}_\mu^\dagger \hat{K}_\mu = \mathbb{1}$. After several measurements, one would like to reconstruct the value of ϑ as well as its standard deviation $\Delta\vartheta$, which gives a reliable quantitative estimate of the determination's precision. If the POVM is fixed, this boils down to a classical problem, where the standard deviation $\Delta\vartheta$ needs to be determined from sampling the conditional distribution $p(\mu|\vartheta) = \mathrm{Tr}(\hat{K}_\mu \varrho_\vartheta \hat{K}_\mu^\dagger)$ of the correlated classical variable μ (the measurement outcome). The solution to this question is given by the classical Fisher information $I_{\hat{K}_\mu,\vartheta}$ (where we emphasise the dependence on the chosen POVM in the context pictured above), given by

$$I_{\hat{K}_\mu,\vartheta} = \sum_\mu p(\mu|\vartheta) \left[\partial_\vartheta \ln\left(p(\mu|\vartheta)\right)\right]^2 = \sum_\mu \frac{\left(p'(\mu|\vartheta)\right)^2}{p(\mu|\vartheta)} \tag{4.1}$$

(where the prime denotes the partial derivative with respect to the parameter ϑ and the summation might be replaced with an integral over a suitable measurable set), and the associated Cramér–Rao bound is

$$\Delta\vartheta \geq \frac{1}{\sqrt{N I_{\hat{K}_\mu,\vartheta}}} , \tag{4.2}$$

where N is the number of measurements carried out. Notice that the lower bound above will in general depend on the value of the parameter ϑ.

The optimisation of the classical Fisher information over all possible POVMs gives rise to the quantum Fisher information I_ϑ:

$$I_\vartheta = \sup_{\hat{K}_\mu} I_{\hat{K}_\mu,\vartheta} \ , \tag{4.3}$$

where, as above, the symbol $\hat{K}_\mu$ stands for the whole POVM, and the associated quantum Cramér–Rao bound:

$$\Delta\vartheta \geq \frac{1}{\sqrt{N I_\vartheta}} \ . \tag{4.4}$$

Since this inequality may be shown to be achievable, it represents the ultimate bound to quantum parameter estimation.

Here, and henceforth, let $\{\varrho_\vartheta\}$ denote the set of states $\Phi_\vartheta(\varrho)$, parameterised by ϑ, in terms of which the estimation problem could have been cast (without reference to the operation Φ_ϑ). Remarkably, the quantum Fisher information of Eq. (4.3) is amenable to the following general characterisation:

$$I_\vartheta = \mathrm{Tr}\left(\varrho_\vartheta \hat{\mathcal{L}}_\vartheta^2\right) \ , \tag{4.5}$$

where the 'symmetric logarithmic derivative' operator is defined implicitly as the self-adjoint operator that satisfies the following equation:

$$2\varrho'_\vartheta = \hat{\mathcal{L}}_\vartheta \varrho_\vartheta + \varrho_\vartheta \hat{\mathcal{L}}_\vartheta \ , \tag{4.6}$$

and thus characterises the sensitivity of the set ϱ_ϑ to variations in the parameter ϑ. Let us note in passing that an equivalent characterisation of the quantum Fisher information may also be given in terms of the 'Bures distance' between quantum states. We will not concern ourselves here with such a connection, but just take the symmetric logarithmic derivative path.

Because of their ready availability, the pervasive nature of Gaussian operations, and their ease of manipulation and description, Gaussian states are obvious, major candidates as metrological probes. This provides a compelling reason for investigating the quantum Fisher information of a set of Gaussian states $\{\varrho_\vartheta\}$, which is the subject of the section to follow.

4.1 Gaussian quantum Fisher information

In order to determine the Fisher information, one has to obtain an expression for the symmetric logarithmic derivative operator $\hat{\mathcal{L}}_\vartheta$, defined in Eq. (4.6). For a set of n-mode Gaussian states ϱ_ϑ, we shall put forward the *ansatz* that the symmetric logarithmic derivative must be at most quadratic, and write (we adopt here and in what follows Einstein's convention of summation over repeated indexes):

$$\hat{\mathcal{L}}_\vartheta = L^{(0)} + L^{(1)}_l \hat{r}_l + L^{(2)}_{jk} \hat{r}_j \hat{r}_k \ , \tag{4.7}$$

where the vector $\hat{\mathbf{r}} = (\hat{x}_1, \hat{p}_1, \ldots, \hat{x}_n, \hat{p}_n)^\mathsf{T}$ is our standard vector of canonical operators, $L^{(0)} \in \mathbb{R}$, $\mathbf{L}^{(1)} \in \mathbb{R}^{2n}$ and $L^{(2)}$ is a symmetric, real $2n \times 2n$ matrix (whose symmetry ensures the overall Hermiticity of the operator).

The methods to determine the operator $\hat{\mathcal{L}}_\vartheta$ will be provided by the characteristic representation, developed in Chapter 2.

Consider in fact the notional operator $\hat{o}$ that admits a characteristic function representation $\chi_{\hat{o}}(\tilde{\mathbf{r}}) = \mathrm{Tr}[\mathrm{e}^{i\tilde{\mathbf{r}}^\mathsf{T}\hat{\mathbf{r}}}\hat{o}]$, where we chose to write the Weyl operator in terms of the variables $\tilde{\mathbf{r}} = \omega\mathbf{r}$. The Baker-Campbell-Hausdorff relation (1.9) may be expressed, in this multivariate setting, as

$$\chi_{\hat{o}}(\tilde{\mathbf{r}}) = \mathrm{Tr}[\mathrm{e}^{i\tilde{\mathbf{r}}^\mathsf{T}\hat{\mathbf{r}}}\hat{o}] = \mathrm{Tr}[\mathrm{e}^{i\tilde{\mathbf{x}}^\mathsf{T}\hat{\mathbf{x}}}\mathrm{e}^{i\tilde{\mathbf{p}}^\mathsf{T}\hat{\mathbf{p}}}\mathrm{e}^{\frac{i}{2}\tilde{\mathbf{x}}^\mathsf{T}\tilde{\mathbf{p}}}\hat{o}] = \mathrm{Tr}[\mathrm{e}^{i\tilde{\mathbf{p}}^\mathsf{T}\hat{\mathbf{p}}}\mathrm{e}^{i\tilde{\mathbf{x}}^\mathsf{T}\hat{\mathbf{x}}}\mathrm{e}^{-\frac{i}{2}\tilde{\mathbf{x}}^\mathsf{T}\tilde{\mathbf{p}}}\hat{o}]\,, \tag{4.8}$$

where we defined the n-dimensional vectors $\hat{\mathbf{x}}$ ($\hat{\mathbf{p}}$) and $\tilde{\mathbf{x}}$ ($\tilde{\mathbf{p}}$) as the vectors of odd (even) entries of the parent vectors $\hat{\mathbf{r}}$ and $\tilde{\mathbf{r}}$, such that $\hat{\mathbf{x}} \oplus \hat{\mathbf{p}} = \hat{\mathbf{r}}$ and $\tilde{\mathbf{x}} \oplus \tilde{\mathbf{p}} = \tilde{\mathbf{r}}$. Now, differentiating the last two equalities of (4.8) yields

$$\partial_{\tilde{p}_j}\chi_{\hat{o}} = i\,\mathrm{Tr}[\mathrm{e}^{i\tilde{\mathbf{r}}^\mathsf{T}\hat{\mathbf{r}}}\hat{o}\,\hat{p}_j] - \frac{i}{2}\tilde{x}_j\chi_{\hat{o}} = i\,\mathrm{Tr}[\mathrm{e}^{i\tilde{\mathbf{r}}^\mathsf{T}\hat{\mathbf{r}}}\hat{p}_j\hat{o}] + \frac{i}{2}\tilde{x}_j\chi_{\hat{o}}\,, \tag{4.9}$$

$$\partial_{\tilde{x}_j}\chi_{\hat{o}} = i\,\mathrm{Tr}[\mathrm{e}^{i\tilde{\mathbf{r}}^\mathsf{T}\hat{\mathbf{r}}}\hat{o}\,\hat{x}_j] + \frac{i}{2}\tilde{p}_j\chi_{\hat{o}} = i\,\mathrm{Tr}[\mathrm{e}^{i\tilde{\mathbf{r}}^\mathsf{T}\hat{\mathbf{r}}}\hat{x}_j\hat{o}] - \frac{i}{2}\tilde{p}_j\chi_{\hat{o}}\,, \tag{4.10}$$

whence

$$\partial_{\tilde{p}_j}\chi_{\hat{o}} = \frac{i}{2}\,\chi_{(\hat{p}_j\hat{o}+\hat{o}\,\hat{p}_j)}\,, \quad \partial_{\tilde{x}_j}\chi_{\hat{o}} = \frac{i}{2}\,\chi_{(\hat{x}_j\hat{o}+\hat{o}\,\hat{x}_j)}\,, \tag{4.11}$$

$$\tilde{p}_j\chi_{\hat{o}} = \chi_{(\hat{x}_j\hat{o}-\hat{o}\,\hat{x}_j)}\,, \quad \tilde{x}_j\chi_{\hat{o}} = -\chi_{(\hat{p}_j\hat{o}-\hat{o}\,\hat{p}_j)}\,. \tag{4.12}$$

Going back to the variables $\tilde{\mathbf{r}}$, the general correspondence between differential or multiplicative terms on the characteristic function and operators can be recast as

$$\partial_{\tilde{r}_j}\chi_{\hat{o}} \longleftrightarrow \frac{i}{2}(\hat{r}_j\hat{o} + \hat{o}\,\hat{r}_j)\,, \quad \tilde{r}_k\chi_{\hat{o}} \longleftrightarrow \Omega_{jk}(\hat{r}_j\hat{o} - \hat{o}\,\hat{r}_j)\,. \tag{4.13}$$

The two relationships (4.13) allow one to bridge between the phase space and the Hilbert space descriptions, and may be applied to the density operator ϱ to establish these correspondences, which will unlock the expression of the quadratic symmetric logarithmic derivative:

$$-2i\partial_{\tilde{r}_j}\chi \leftrightarrow \hat{r}_j\varrho + \varrho\hat{r}_j\,, \tag{4.14}$$

$$\frac{1}{2}(\Omega_{jj'}\tilde{r}_{j'}\Omega_{kk'}\tilde{r}_{k'} - 4\partial_{\tilde{r}_k}\partial_{\tilde{r}_j})\chi \leftrightarrow \hat{r}_k\hat{r}_j\varrho + \varrho\hat{r}_j\hat{r}_k\,. \tag{4.15}$$

Since the variables $\tilde{r}_j$ are defined as $\Omega_{jj'}r_{j'}$, the characteristic function χ_G of a generic Gaussian state with covariance matrix $\boldsymbol{\sigma}$ and first moments $\mathbf{d}$, that both depend on ϑ, can be written as

$$\chi_G = \mathrm{e}^{-\frac{1}{4}\sigma_{jk}\tilde{r}_j\tilde{r}_k + i\tilde{r}_l d_l}\,, \tag{4.16}$$

whence

$$\partial_{\tilde{r}_j}\chi_G = \left(id_j - \frac{1}{2}\sigma_{jj'}\tilde{r}_{j'}\right)\chi_G \,, \tag{4.17}$$

$$\partial_{\tilde{r}_k}\partial_{\tilde{r}_j}\chi_G = \left[\left(id_k - \frac{1}{2}\sigma_{kk'}\tilde{r}_{k'}\right)\left(id_j - \frac{1}{2}\sigma_{jj'}\tilde{r}_{j'}\right) - \frac{1}{2}\sigma_{jk}\right]\chi_G \,, \tag{4.18}$$

$$\chi_G' = \left(i\tilde{r}_p d_p' - \frac{1}{4}\sigma_{lm}'\tilde{r}_l\tilde{r}_m\right)\chi_G \,, \tag{4.19}$$

where a prime $'$ stands for the derivative with respect to the estimation parameter ϑ. Eqs. (4.7), (4.14) and (4.15) allow one to rephrase the symmetric logarithmic derivative equation (4.6) as the following condition:

$$\begin{aligned} 2i\tilde{r}_p d_p' - \frac{\sigma_{lm}'}{2}\tilde{r}_l\tilde{r}_m =& 2L^{(0)} + L_p^{(1)}\left(2d_p + i\sigma_{pp'}\tilde{r}_{p'}\right) + L_{jk}^{(2)}\big(\frac{\Omega_{jj'}\tilde{r}_{j'}\Omega_{kk'}\tilde{r}_{k'}}{2} \\ & - \frac{\sigma_{jj'}\tilde{r}_{j'}\sigma_{kk'}\tilde{r}_{k'}}{2} + \sigma_{jk} + 2d_j d_k + id_j\sigma_{kk'}\tilde{r}_{k'} + id_k\sigma_{jj'}\tilde{r}_{j'}\big) \end{aligned} \tag{4.20}$$

(we have divided by χ_G, which is allowed since it is never zero). This must hold for all $\tilde{\mathbf{r}}$, so that we can equate the different orders of the last equation independently. It is convenient to switch back to a geometric representation of the matrices involved, without indexes, to find

$$\boldsymbol{\sigma}' = \boldsymbol{\sigma}L^{(2)}\boldsymbol{\sigma} + \Omega L^{(2)}\Omega \,, \tag{4.21}$$

$$\mathbf{L}^{(1)} = 2\boldsymbol{\sigma}^{-1}\mathbf{d}' - 2L^{(2)}\mathbf{d} \,, \tag{4.22}$$

$$L^{(0)} = -\frac{1}{2}\mathrm{Tr}[\boldsymbol{\sigma}L^{(2)}] - \mathbf{L}^{(1)\mathsf{T}}\mathbf{d} - \mathbf{d}^{\mathsf{T}}L^{(2)}\mathbf{d} \,. \tag{4.23}$$

Note that $A_{jk}B_{jk} = \mathrm{Tr}[AB]$, which is just the Hilbert–Schmidt inner product if A and B are real and symmetric. Notice also that, in keeping with our general notation, $\mathbf{L}^{(1)}$ stands for the vector with components $L_j^{(1)}$. Once $L^{(2)}$ is determined by Eq. (4.21), $\mathbf{L}^{(1)}$ and $L^{(0)}$ are given by Eqs. (4.22) and (4.23).

In order to determine $L^{(2)}$, we need to analyse the linear functional $\mathcal{A}_{\boldsymbol{\sigma}}$ that maps real matrices into matrices according to $\mathcal{A}_{\boldsymbol{\sigma}}(M) = \boldsymbol{\sigma}M\boldsymbol{\sigma} + \Omega M\Omega$. Clearly, if $\mathcal{A}_{\boldsymbol{\sigma}}$ were invertible, one would have $\mathcal{A}_{\boldsymbol{\sigma}}^{-1}(\boldsymbol{\sigma}')$. The inverse $\mathcal{A}_{\boldsymbol{\sigma}}^{-1}$ may be obtained fairly easily by the symplectic diagonalisation of $\boldsymbol{\sigma}$. In fact, let S^{-1} be the symplectic that turns $\boldsymbol{\sigma}$ in normal form such that, without loss of generality, $\boldsymbol{\sigma} = S\boldsymbol{\nu}S^{\mathsf{T}}$ with $\boldsymbol{\nu} = \bigoplus_{j=1}^{n}\nu_j\mathbb{1}_2$. Then, one has

$$\mathcal{A}_{\boldsymbol{\sigma}}(M) = S\left(\boldsymbol{\nu}S^{\mathsf{T}}MS\boldsymbol{\nu} + \Omega S^{\mathsf{T}}MS\Omega\right)S^{\mathsf{T}} = S\mathcal{A}_{\boldsymbol{\nu}}(S^{\mathsf{T}}MS)S^{\mathsf{T}} \,, \tag{4.24}$$

where we used the symplectic conditions $S^{-1}\Omega = \Omega S^{\mathsf{T}}$ and $\Omega S^{\mathsf{T}-1} = S\Omega$. The inverse of the map $\mathcal{A}_{\boldsymbol{\sigma}}$, which we are aiming for, may hence be written as

$$\mathcal{A}_{\boldsymbol{\sigma}}^{-1}(M) = S^{\mathsf{T}-1}\mathcal{A}_{\boldsymbol{\nu}}^{-1}(S^{-1}MS^{\mathsf{T}-1})S^{-1} \,. \tag{4.25}$$

Now, the maps $\Omega\cdot\Omega = -\Omega\cdot\Omega^{\mathsf{T}}$ and $\boldsymbol{\nu}\cdot\boldsymbol{\nu}$, given by the congruence action of two block matrices, one of which has all blocks proportional to the identity, clearly commute: $\boldsymbol{\nu}\Omega M\Omega\boldsymbol{\nu} = \Omega\boldsymbol{\nu}M\boldsymbol{\nu}\Omega$. A set $\mathfrak{A}$ of common 'eigenmatrices' for such maps is promptly seen to be the following:

$$\begin{aligned}\mathfrak{A} &= \frac{1}{\sqrt{2}}\{\Omega_1^{(jk)},\ \sigma_z^{(jk)},\ \mathbb{1}_2^{(jk)},\ \sigma_x^{(jk)}\ ,\ j,k\in[1,\ldots,n]\}\\ &= \{A_l^{(jk)}\ ,\ l\in[0,\ldots,3]\ ,\ j,k\in[1,\ldots,n]\}\ ,\end{aligned} \tag{4.26}$$

where the superscript $^{(jk)}$ indicates that the matrix is zero everywhere except for the 2×2 block in position jk, whose entries equal the indicated matrix (recall that Ω_1 stands the single-mode symplectic form Ω, while σ_z and σ_x are standard Pauli matrices). It is easy to verify that $\Omega\cdot\Omega$ has eigenvalue -1 for $\mathbb{1}_2^{(jk)}$ and $\Omega_1^{(jk)}$ and $+1$ for $\sigma_z^{(jk)}$ and $\sigma_x^{(jk)}$, whilst $\boldsymbol{\nu}$ has eigenvalue $\nu_j\nu_k$ for each eigenmatrix with superscript $^{(jk)}$. Besides, the eigenmatrices above have been chosen so that they are orthonormal with respect to the Hilbert–Schmidt inner product.

The eigenvalues of the map $\mathcal{A}_{\boldsymbol{\nu}}$ are hence $\nu_j\nu_k\mp 1$ (each of the eigenmatrices $M_l^{(jk)}$, ordered as per Eq. (4.26), has associated eigenvalue $(\nu_j\nu_k-(-1)^l)$). Such a map is therefore invertible if and only if $\nu_j\neq 1$ for all j, that is, if all the local states of the normal modes of the global state with covariance matrix $\boldsymbol{\sigma}$ are mixed. If any such state is pure, with $\nu_j = 1$, then the full inversion of the map $\mathcal{A}_{\boldsymbol{\nu}}$, and hence $\mathcal{A}_{\boldsymbol{\sigma}}$, is generally not possible (notice that the inversions of symplectic matrices that occur in the relationship between the two maps are always possible since $\mathrm{Det}S = 1$: no issue may arise there). Even then, the matrix $L^{(2)}$ may still be determined, according to Eq. (4.21), if the argument $\boldsymbol{\sigma}'$ is orthogonal to the singular eigenvalues. As we will see in detail in the next section in the case of a single mode, this is equivalent to stating that a change in the parameter ϑ is not able to turn the pure state with covariance matrix $\boldsymbol{\sigma}$ into a mixed state: if that is the case, the symmetric logarithmic derivative, and hence the quantum Fisher information, are still well defined. At a more fundamental, mathematical level, this is a reflection of the fact that turning a pure state into a mixed one means suddenly changing the rank of the state (incidentally, in the Gaussian case, the rank jumps from 1 to ∞, as Gaussian states admit only such two values for the rank): when that happens, the symmetric logarithmic derivative operator may not exist. Although this clarification was in order, we will now proceed assuming the inverse $\mathcal{A}_{\boldsymbol{\sigma}}^{-1}$ exists: pathological cases related to the singularity of $\mathcal{A}_{\boldsymbol{\sigma}}$ will emerge at the end of our discussion as divergences in the quantum Fisher information. Formally, our treatment will be equivalent to perturbing slightly, by a quantity ϵ, the incriminated symplectic eigenvalues, and then determining the limit $\epsilon\to 0$ at the end of the evaluation. Notice also that the case $\nu_j+\epsilon$ is indistinguishable from ν_j for all practical purposes.

We can then proceed to invert Eq. (4.21) and write

$$L^{(2)} = \mathcal{A}_{\boldsymbol{\sigma}}^{-1}(\boldsymbol{\sigma}')\ . \tag{4.27}$$

In a practical calculation, given $\boldsymbol{\sigma}'$ and $\boldsymbol{\sigma} = S\boldsymbol{\nu}S^{\mathsf{T}}$, one would simply parametrise the matrix $S^{-1}\boldsymbol{\sigma}'S^{\mathsf{T}-1}$ as a superposition of eigenmatrices:

$$S^{-1}\boldsymbol{\sigma}'S^{\mathsf{T}-1} = a_l^{(jk)} A_l^{(jk)} \ , \tag{4.28}$$

and then explicitly have

$$L^{(2)} = \mathcal{A}_{\boldsymbol{\sigma}}^{-1}(\boldsymbol{\sigma}') = \frac{a_l^{(jk)}}{\nu_j\nu_k - (-1)^l} S^{\mathsf{T}-1} A_l^{(jk)} S^{-1} \ . \tag{4.29}$$

Now that we have obtained a formula for the Gaussian symmetric logarithmic derivative $\hat{\mathcal{L}}_\vartheta$, we can proceed to insert it into the expression for the quantum Fisher information (4.5). This task is simplified by noticing that Eqs. (4.6) and (4.5) may be combined to obtain the following expression for the quantum Fisher information

$$I_\vartheta = \mathrm{Tr}[\varrho'_\vartheta \hat{\mathcal{L}}_\vartheta] \ , \tag{4.30}$$

and that we already know the characteristic function associated with ϱ'_ϑ, which is nothing but χ'_G of Eq. (4.19). From Eqs. (4.13) we know that the characteristic function $\chi_{\hat{o}\hat{r}_j}$ associated with operator $\hat{o}\hat{r}_j$ may be derived from the characteristic function $\chi_{\hat{o}}$ associated with operator $\hat{o}$ as $\chi_{\hat{o}\hat{r}_j} = (-i\partial_{\tilde{r}_j} - \frac{1}{2}\Omega_{jj'}\tilde{r}_{j'})\chi_{\hat{o}}$. We can then apply the powerful property of the characteristic function whereby the expectation value of the associated operator is just the characteristic function evaluated in 0, to obtain, recalling the quadratic form (4.7):

$$\begin{aligned} I_\vartheta =& \mathrm{Tr}[\varrho'_\vartheta \hat{\mathcal{L}}_\vartheta] = \Big[L^{(0)} + L_j^{(1)}(-i\partial_{\tilde{r}_j} - \frac{1}{2}\Omega_{jj'}\tilde{r}_{j'}) \\ &+ L_{jk}^{(2)}(-i\partial_{\tilde{r}_k} - \frac{1}{2}\Omega_{kk'}\tilde{r}_{k'})(-i\partial_{\tilde{r}_j} - \frac{1}{2}\Omega_{jj'}\tilde{r}_{j'}) \Big] \left(i\tilde{r}_p d'_p - \frac{1}{4}\sigma'_{lm}\tilde{r}_l\tilde{r}_m \right) \chi_G \Big|_{\tilde{\mathbf{r}}=0} \\ =& L_j^{(1)} d'_j + \frac{1}{2} L_{jk}^{(2)} \sigma'_{jk} + 2 L_{jk}^{(2)} d'_j d_k \ , \end{aligned} \tag{4.31}$$

which, going back to a geometric notation, without indexes, and replacing $\mathbf{L}^{(1)}$ with its expression (4.22), becomes

$$I_\vartheta = \frac{1}{2}\mathrm{Tr}[L^{(2)}\boldsymbol{\sigma}'] + 2\mathbf{d}'^{\mathsf{T}}\boldsymbol{\sigma}^{-1}\mathbf{d}' \ . \tag{4.32}$$

It is certainly worthwhile to summarise our findings as follows:

Gaussian quantum Fisher information. Given a set of Gaussian states with covariance matrix $\boldsymbol{\sigma}_\vartheta$ and first moments $\mathbf{d}_\vartheta$ depending on one real parameter ϑ, the quantum Fisher information I_ϑ associated with the optimal estimation of ϑ may be determined as follows:

1. Determine the normal mode decomposition $\boldsymbol{\sigma}_\vartheta = S\left(\bigoplus_{j=1}^n \nu_j \mathbb{1}_2\right) S^\mathsf{T}$.
2. Evaluate the matrix $S^{-1}\boldsymbol{\sigma}'S^{\mathsf{T}-1}$, where $\boldsymbol{\sigma}' = \partial_\vartheta \boldsymbol{\sigma}_\vartheta$, and determine the coefficients $a_l^{(jk)} = \mathrm{Tr}[A_l^{(jk)} S^{-1}\boldsymbol{\sigma}'S^{\mathsf{T}-1}]$, where $A_l^{(jk)}$ are the basis matrices defined in Eq. (4.26), such that $S^{-1}\boldsymbol{\sigma}'S^{\mathsf{T}-1} = a_l^{(jk)} A_j^{(jk)}$.
3. Evaluate the matrix $L^{(2)} = \frac{a_l^{(jk)}}{\nu_j\nu_k - (-1)^l} S^{\mathsf{T}-1} A_l^{(jk)} S^{-1}$.
4. Evaluate $I_\vartheta = \frac{1}{2}\mathrm{Tr}[L^{(2)}\boldsymbol{\sigma}'] + 2\mathbf{d}'^\mathsf{T}\boldsymbol{\sigma}_\vartheta^{-1}\mathbf{d}'$, where $\mathbf{d}' = \partial_\vartheta \mathbf{d}_\vartheta$.

The optimal measurement to be carried out in order to attain the quantum Cramér–Rao bound is the projective von Neumann measurement in the basis which diagonalises the symmetric logarithmic derivative and may also be worked out by determining the normal mode decomposition of the matrix $L^{(2)}$, associated with the quadratic operator $\hat{\mathcal{L}}_\vartheta$ through Eq. (4.7). It will hence correspond to a number measurement in the Fock basis that diagonalises $\hat{\mathcal{L}}_\vartheta$.

Note that we have not dealt with the possibility of multi-parameter estimation, where the Cramér–Rao bound turns into a matrix inequality on the error covariance matrix, nor have we discussed the problem of choosing input probe states, on which the estimation of a partially unknown quantum operation will in general strongly depend. In the following section, we will specialise our treatment to the single-mode case and show some examples that should provide the reader with some intuition as to how the findings above apply in practical cases.

4.2 Quantum estimation with single-mode Gaussian states

The reduction of the general recipe above to single-mode states is both very instructive and extremely relevant to applications. Single-mode states enjoy the specificity of possessing a single symplectic eigenvalue ν_1, so that $\boldsymbol{\sigma} = SS^\mathsf{T}\nu_1$.[1] Let us now expand the generic matrix $S^{-1}\boldsymbol{\sigma}'S^{\mathsf{T}-1}$ in the basis of Eq. (4.26), comprising the three matrices $\mathbb{1}_2$, σ_z and σ_x (Ω_1 is redundant here, since $S^{-1}\boldsymbol{\sigma}'S^{\mathsf{T}-1}$ is symmetric):

$$S^{-1}\boldsymbol{\sigma}'S^{\mathsf{T}-1} = a_1\frac{\sigma_z}{\sqrt{2}} + a_2\frac{\mathbb{1}_2}{\sqrt{2}} + a_3\frac{\sigma_x}{\sqrt{2}}\,, \tag{4.33}$$

[1] In fact, the argument developed in this section could be generalised to 'isotropic' multi-mode states – with fully degenerate symplectic spectrum – for which the same identity holds, since the symplectic transformation can be carried through the normal mode form (which is proportional to the identity for such states).

in terms of the three generic real coefficients a_1, a_2 and a_3. Notice that this implies

$$\boldsymbol{\sigma}' = S\left(a_1\frac{\sigma_z}{\sqrt{2}} + a_2\frac{\mathbb{1}_2}{\sqrt{2}} + a_3\frac{\sigma_x}{\sqrt{2}}\right)S^{\mathsf{T}} \,. \tag{4.34}$$

The following expression for $L^{(2)}$ immediately ensues:

$$L^{(2)} = S^{\mathsf{T}-1}\left(\frac{a_1}{\nu_1^2+1}\frac{\sigma_z}{\sqrt{2}} + \frac{a_2}{\nu_1^2-1}\frac{\mathbb{1}_2}{\sqrt{2}} + \frac{a_3}{\nu_1^2+1}\frac{\sigma_x}{\sqrt{2}}\right)S^{-1} \,. \tag{4.35}$$

The evaluation of Eq. (4.32) is now made straightforward by the fact that the eigenmatrices we have chosen are orthonormal with respect to the Hilbert–Schmidt scalar product, which is precisely what needs to be computed between $L^{(2)}$ and $\boldsymbol{\sigma}'$. One then gets (note that similarity transformations preserve the trace)

$$I_\vartheta = \frac{1}{2}\left(\frac{a_1^2}{\nu_1^2+1} + \frac{a_2^2}{\nu_1^2-1} + \frac{a_3^2}{\nu_1^2+1}\right) + 2\mathbf{d}'^{\mathsf{T}}\boldsymbol{\sigma}^{-1}\mathbf{d}' \,. \tag{4.36}$$

This equation may be recast in a more direct and appealing form, by singling out the effect of the change in parameter on the purity $\mu = \mathrm{Tr}(\varrho_\vartheta^2)$ of the Gaussian states under scrutiny. For Gaussian states of one mode, we know that $\mu = 1/\sqrt{\mathrm{Det}\boldsymbol{\sigma}} = \nu_1^{-1}$. Furthermore, $\boldsymbol{\sigma}^{-1} = S^{\mathsf{T}-1}S^{-1}\nu_1^{-1}$. By evaluating $\mathrm{Det}(\boldsymbol{\sigma} + \boldsymbol{\sigma}'\mathrm{d}\vartheta)$ at first order in $\mathrm{d}\vartheta$, it is easy to verify that $(\mathrm{Det}\boldsymbol{\sigma})' = \mathrm{Tr}[\boldsymbol{\sigma}^{-1}\boldsymbol{\sigma}']\mathrm{Det}\boldsymbol{\sigma} = \sqrt{2}\nu_1 a_2$, where we used Eq. (4.34) for $\boldsymbol{\sigma}'$. In terms of the purity μ, one has $\mu' = -\frac{1}{2}\frac{(\mathrm{Det}\boldsymbol{\sigma})'}{(\mathrm{Det}\boldsymbol{\sigma})^{3/2}} = -\frac{a_2\mu^2}{\sqrt{2}}$.

Notice now that

$$\begin{aligned}\mathrm{Tr}[(\boldsymbol{\sigma}^{-1}\boldsymbol{\sigma}')^2] &= \mu^2(a_1^2+a_2^2+a_3^2)\\ &= \mu^2(1+\mu^2)\left(\frac{a_1^2}{1+\mu^2} + \frac{a_2^2}{1-\mu^2} + \frac{a_3^2}{1+\mu^2}\right) - \frac{2\mu^4 a_2^2}{1-\mu^2}\\ &= \mu^2(1+\mu^2)\left(\frac{a_1^2}{1+\mu^2} + \frac{a_2^2}{1-\mu^2} + \frac{a_3^2}{1+\mu^2}\right) - \frac{4\mu'^2}{1-\mu^2} \,,\end{aligned} \tag{4.37}$$

which can be inserted into Eq. (4.36), recalling that $\nu_1 = \mu^{-1}$, to obtain the following notable result:

Single-mode Gaussian quantum Fisher information. The quantum Fisher information I_ϑ of a set of single-mode Gaussian states with covariance matrices $\boldsymbol{\sigma}_\vartheta$ and first moments $\mathbf{d}_\vartheta$ is given by

$$I_\vartheta = \frac{1}{2}\frac{\mathrm{Tr}[(\boldsymbol{\sigma}^{-1}\boldsymbol{\sigma}')^2]}{1+\mu^2} + \frac{2\mu'^2}{1-\mu^4} + 2\mathbf{d}'^{\mathsf{T}}\boldsymbol{\sigma}^{-1}\mathbf{d}' \,, \tag{4.38}$$

where $\mu = 1/\sqrt{\mathrm{Det}\boldsymbol{\sigma}_\vartheta}$ is the purity of the quantum states and the prime $'$ denotes differentiation with respect to the parameter ϑ.

Notice that this parametrisation clearly isolates the term that may lead to diverging Fisher information as the one dependent on the derivative of the

purity. As discussed in the previous section, this is related to the impossibility of defining the symmetric logarithmic derivative and is due to the fact that such a term would be responsible for a sudden change in the rank of the Gaussian state, jumping from 1 to ∞.