Supporting Information for: Holographic Gaussian Boson Sampling with Matrix Product States on 3D cQED Processors

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1 Representations of the Gaussian state

The goal of this section is to first introduce the eigenstates of the annihilation operator, the so-called coherent states $|\alpha\rangle$ that fulfill the eigenvalue equation

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle, \tag{S1}$$

where $\alpha \in \mathbb{C}$ is a given complex number. Based on the coherent states, we will then introduce the so called P-representation of density operators that we will use to unfold GBS. We will see that a coherent state has a precise phase defined by the complex amplitude α, although an indefinite number of photons, like the state of coherent light in a laser beam. In contrast, a Fock state is an eigenstate of the number operator, corresponding to a fixed well-defined number of photons although completely arbitrary (random) phase. In the following, we focus on harmonic oscillator coherent states, while noting that generalization to anharmonic coherent states is readily available.[1]

1.1 Overview of the coherent states

The goal of this subsection is to provide an overview of properties of coherent states that would be vital for applications to the GBS.

Displacement operator. We start by showing that we can create coherent states, as follows

$$\hat{D}(\alpha)|0\rangle = |\alpha\rangle, \tag{S2}$$

where $|0\rangle$ is the vacuum state defined as the ground state of the harmonic oscillator, and $\hat{D}(\alpha)$ is the displacement operator, defined as follows

$$\begin{aligned} \hat{D}(\alpha) &= e^{\alpha \hat{a}^\dagger - \alpha^* \hat{a}} \\ &= e^{\alpha \hat{a}^\dagger} e^{-\alpha^* \hat{a}} e^{-\frac{1}{2}|\alpha|^2}. \end{aligned} \tag{S3}$$

The second row of Eq. (S3) is obtained from the first one by using the Hausdorff formula $e^{\hat{A}+\hat{B}} = e^{\hat{A}} e^{\hat{B}} e^{-\frac{1}{2}[\hat{A},\hat{B}]}$, with $\hat{A} = \alpha \hat{a}^\dagger$ and $\hat{B} = -\alpha^* \hat{a}$, which is valid if $[\hat{A},[\hat{A},\hat{B}]] = [\hat{B},[\hat{A},\hat{B}]] = 0$, as in this case. Note that $[\hat{A},\hat{B}] = -|\alpha|^2[\hat{a}^\dagger,\hat{a}] = |\alpha|^2$, since $[\hat{a}^\dagger,\hat{a}] = -1$.

We will obtain Eqs. (S1) and (S2) by showing that, according to the Baker–Campbell–

Hausdorff relation, $\hat{D}(\alpha)^\dagger \hat{a}\hat{D}(\alpha) = \hat{a} + \alpha$ (part 1). Hence, with $\hat{a}|0\rangle = 0$, we can conclude that $\hat{D}(\alpha)^\dagger \hat{a}\hat{D}(\alpha)|0\rangle = \alpha|0\rangle$, and $\hat{a}\hat{D}(\alpha)|0\rangle = \alpha\hat{D}(\alpha)|0\rangle$ (part 2). Consequently, by definition, $\hat{D}(\alpha)|0\rangle$ is equal to $|\alpha\rangle$: the eigenfunction of $\hat{a}$ with eigenvalue α.

Let us start with part 1: Firstly, we show that $\hat{D}(\alpha)^{-1} = \hat{D}(-\alpha) = \hat{D}(\alpha)^\dagger$:

$$\begin{aligned} \hat{D}(\alpha)^{-1} &= e^{\frac{1}{2}|\alpha|^2} e^{\alpha^* \hat{a}} e^{-\alpha \hat{a}^\dagger} \\ &= e^{-\frac{1}{2}|\alpha|^2} e^{-\alpha \hat{a}^\dagger} e^{\alpha^* \hat{a}} = \hat{D}(-\alpha), \end{aligned} \tag{S4}$$

where the first equality follows from $\hat{D}(\alpha)^{-1}\hat{D}(\alpha) = 1$. The second row of Eq. (S4) is obtained from the first one since

$$e^{\alpha^* \hat{a}} e^{-\alpha \hat{a}^\dagger} = e^{-\alpha \hat{a}^\dagger} e^{\alpha^* \hat{a}} e^{-|\alpha|^2}. \tag{S5}$$

The Baker–Campbell–Hausdorff relation

$$e^{\hat{A}} \hat{B} e^{-\hat{A}} = \hat{B} + [\hat{A}, \hat{B}] + \frac{1}{2}[\hat{A}, [\hat{A}, \hat{B}]] + \dots \tag{S6}$$

can be used with $\hat{A} = -\alpha \hat{a}^\dagger + \alpha^* \hat{a}$, and $\hat{B} = \hat{a}$ to show that

$$\hat{D}(\alpha)^\dagger \hat{a} \hat{D}(\alpha) = \hat{a} + \alpha, \tag{S7}$$

since $[\hat{A}, \hat{B}] = [-\alpha \hat{a}^\dagger + \alpha^* \hat{a}, \hat{a}] = \alpha$, and therefore $[\hat{A}, [\hat{A}, \hat{B}]] = 0$. For part 2, we apply the vacuum state $|0\rangle$ to Eq. (S7) and obtain

$$\hat{D}(\alpha)^\dagger \hat{a} \hat{D}(\alpha)|0\rangle = \alpha|0\rangle, \tag{S8}$$

since we have $\hat{a}|0\rangle = 0$. Therefore, according to Eq. (S1), we conclude that

$$\hat{D}(\alpha)|0\rangle = |\alpha\rangle, \tag{S9}$$

which indeed is Eq. (S2).

Series expansion. Substituting Eq. (S3) into Eq. (S9), we obtain

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} e^{\alpha\hat{a}^\dagger} e^{-\alpha^*\hat{a}}|0\rangle \tag{S10}$$

and by expanding the exponentials in Taylor series, we get

$$\begin{aligned} |\alpha\rangle &= e^{-\frac{1}{2}|\alpha|^2} e^{\alpha\hat{a}^\dagger}|0\rangle \\ &= e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{n!} (\hat{a}^\dagger)^n |0\rangle \\ &= e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle, \end{aligned} \tag{S11}$$

where the third row is obtained by $\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$. In particular, we obtain the following eigenvalue equation $\hat{a}|\alpha\rangle = \alpha|\alpha\rangle$ since

$$\begin{aligned} \hat{a}|\alpha\rangle &= e^{-\frac{1}{2}|\alpha|^2} \sum_{n=1}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \sqrt{n}|n-1\rangle \\ &= e^{-\frac{1}{2}|\alpha|^2} \sum_{n=1}^{\infty} \alpha \frac{\alpha^{n-1}}{\sqrt{(n-1)!}} |n-1\rangle \\ &= \alpha e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{(n)!}} |n\rangle. \end{aligned} \tag{S12}$$

Given that the coherent state is an eigenstate of the annihilation operator, its complex conjugate is an eigenstate of the creation operator

$$(\hat{a}\,|\alpha\rangle)^{\dagger} = (\alpha\,|\alpha\rangle)^{\dagger}\,, \tag{S13}$$

$$\langle\alpha|\,\hat{a}^{\dagger} = \langle\alpha|\,\alpha^{\star}. \tag{S14}$$

Overlap. Coherent states are not orthogonal since, according to Eq. (S11),

$$\begin{aligned}\langle\beta|\alpha\rangle &= e^{-\frac{1}{2}|\alpha|^2} e^{-\frac{1}{2}|\beta|^2} \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \frac{(\beta^*)^m \alpha^n}{\sqrt{m!n!}} \langle m|n\rangle \\ &= e^{-\frac{1}{2}|\alpha|^2} e^{-\frac{1}{2}|\beta|^2} \sum_{n=0}^{\infty} \frac{(\beta^*)^n \alpha^n}{n!} \\ &= e^{-\frac{1}{2}|\alpha|^2} e^{-\frac{1}{2}|\beta|^2} e^{\beta^*\alpha} \\ &= e^{-\frac{1}{2}|\beta-\alpha|^2} e^{\frac{1}{2}(\beta^*\alpha - \beta\alpha^*)}\end{aligned} \tag{S15}$$

Expectation values. The expectation value of position,

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(a + a^{\dagger}\right), \tag{S16}$$

follows from

$$\langle\alpha\,|\hat{x}|\,\alpha\rangle = \left\langle\alpha\left|\sqrt{\frac{\hbar}{2m\omega}}\left(a + a^{\dagger}\right)\right|\alpha\right\rangle \tag{S17}$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left(\langle\alpha\,|a|\,\alpha\rangle + \left\langle\alpha\,\middle|a^{\dagger}\middle|\,\alpha\right\rangle\right) \tag{S18}$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left(\alpha\,\langle\alpha|\alpha\rangle + \alpha^{\star}\,\langle\alpha|\alpha\rangle\right) \tag{S19}$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left(\alpha + \alpha^{\star}\right) \tag{S20}$$

$$= \sqrt{\frac{2\hbar}{m\omega}}\,\mathrm{Re}\left(\alpha\right). \tag{S21}$$

Likewise, the expectation value of the momentum,

$$\hat{p} = -i\sqrt{\frac{m\hbar\omega}{2}}\left(a - a^{\dagger}\right), \tag{S22}$$

follows from

$$\langle \alpha \left| \hat{p} \right| \alpha \rangle = \left\langle \alpha \left| -i\sqrt{\frac{m\hbar\omega}{2}}\left(a - a^{\dagger}\right) \right| \alpha \right\rangle \tag{S23}$$

$$= -i\sqrt{\frac{m\hbar\omega}{2}}\left(\langle \alpha \left| a \right| \alpha \rangle - \left\langle \alpha \left| a^{\dagger} \right| \alpha \right\rangle\right) \tag{S24}$$

$$= -i\sqrt{\frac{m\hbar\omega}{2}}\left(\alpha \langle \alpha | \alpha \rangle - \alpha^{\star} \langle \alpha | \alpha \rangle\right) \tag{S25}$$

$$= -i\sqrt{\frac{m\hbar\omega}{2}}\left(\alpha - \alpha^{\star}\right) \tag{S26}$$

$$= \sqrt{2m\hbar\omega}\,\mathrm{Im}\left(\alpha\right). \tag{S27}$$

Therefore, according to Eq. (S17) and Eq. (S23), we obtain

$$\alpha = \alpha_r + i\alpha_i = \sqrt{\frac{m\omega}{2\hbar}} q_{\alpha} + i\frac{1}{\sqrt{2m\hbar\omega}} p_{\alpha}, \tag{S28}$$

where $q_{\alpha} = \langle \alpha | \hat{x} | \alpha \rangle$ and $p_{\alpha} = \langle \alpha | \hat{p} | \alpha \rangle$.

Representation as wavefunction. The wavefunctions can be obtain by substituting the eigenfunctions of the Harmonic oscillator,

$$\langle x | n \rangle = (2^n n!)^{-1/2}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\tilde{x}^2/2\right) H_n(\tilde{x}), \tag{S29}$$

into Eq. (S11), where $\tilde{x} = x\sqrt{m\omega/\hbar}$, with H_n the nth-Hermite polynomial, giving

$$\langle x | \alpha \rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{1}{2}|\alpha|^2} e^{-\frac{1}{2}\tilde{x}^2} \sum_{n=0}^{\infty} \frac{(\alpha/\sqrt{2})^n}{n!} H_n(\tilde{x}). \tag{S30}$$

The vacuum state corresponding to $n = 0$ photons is described by the wavefunction $\langle x|0\rangle$. According to Eq. (S30), $\langle x|0\rangle$ is also a coherent state with $\alpha = 0$ (*i.e.*, the ground state of a harmonic oscillator with mass m and frequency ω). We note that the Hermite polynomials are given by the characteristic function

$$e^{2\tilde{x}t-t^2} = \sum_{n=0}^{\infty} H_n(\tilde{x})\frac{t^n}{n!}, \tag{S31}$$

as can be verified by the Taylor expansion at $\tilde{x}$. Therefore, substituting the characteristic function into Eq. (S30), with $t = \alpha/\sqrt{2}$, we obtain

$$\begin{aligned}
\langle x|\alpha\rangle &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{1}{2}|\alpha|^2} e^{\frac{1}{2}\tilde{x}^2} e^{-(\tilde{x}-\alpha/\sqrt{2})^2} \\
&= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{1}{2}(\alpha_r^2+\alpha_i^2)} e^{\frac{1}{2}\tilde{x}^2} e^{-(\tilde{x}-\alpha_r/\sqrt{2}-i\alpha_i/\sqrt{2})^2} \\
&= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{1}{2}(\alpha_r^2+\alpha_i^2)} e^{\frac{1}{2}\tilde{x}^2} e^{-(\tilde{x}^2+\alpha_r^2/2-\alpha_i^2/2+i\alpha_r\alpha_i-\sqrt{2}\tilde{x}(\alpha_r+i\alpha_i))} \\
&= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\alpha_r^2} e^{-\frac{1}{2}\tilde{x}^2} e^{\sqrt{2}\tilde{x}\alpha_r} e^{-i\alpha_i(\alpha_r-\sqrt{2}\tilde{x})} \\
&= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-(\alpha_r-\tilde{x}/\sqrt{2})^2} e^{-i\alpha_i(\alpha_r-\sqrt{2}\tilde{x})}.
\end{aligned} \tag{S32}$$

Substituting α_r and α_i in terms of q_α and p_α, we obtain

$$\begin{aligned}
\langle x|\alpha\rangle &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\left(q_\alpha\sqrt{\frac{m\omega}{2\hbar}}-x\sqrt{\frac{m\omega}{2\hbar}}\right)^2} e^{-ip_\alpha\sqrt{\frac{1}{2m\hbar\omega}}\left(q_\alpha\sqrt{\frac{m\omega}{2\hbar}}-\sqrt{2}x\sqrt{\frac{m\omega}{\hbar}}\right)} \\
&= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\left(\frac{m\omega}{2\hbar}\right)(x-q_\alpha)^2} e^{\frac{i}{\hbar}p_\alpha(x-q_\alpha)} e^{\frac{i}{2\hbar}p_\alpha q_\alpha} \\
&= \left(\frac{\gamma}{\pi}\right)^{1/4} e^{-\frac{\gamma}{2}(x-q_\alpha)^2} e^{\frac{i}{\hbar}p_\alpha(x-q_\alpha)} e^{\frac{i}{2\hbar}p_\alpha q_\alpha},
\end{aligned} \tag{S33}$$

with $\gamma = m\omega/\hbar$.

1.2 P-representation of the density operator

The Glauber-Sudarshan P-representation of the density operator, $\hat{\rho}$ (*i.e.*, the P-function, $P(\alpha)$), is a pseudo-probability distribution defined, as follows

$$\hat{\rho} = \int P(\alpha)|\alpha\rangle\langle\alpha|\, \mathrm{d}^2\alpha, \tag{S34}$$

where $\mathrm{d}^2\alpha = \mathrm{d}\,\mathrm{Re}(\alpha)\mathrm{d}\,\mathrm{Im}(\alpha)$. As shown below,

$$P(\alpha) = \frac{e^{|\alpha|^2}}{\pi^2} \int e^{-\alpha^* u + u^* \alpha} \langle -u|\hat{\rho}|u\rangle e^{|u|^2}\, \mathrm{d}^2 u. \tag{S35}$$

To prove Eq. (S35), we follow Mehta and compute $\langle -u|\hat{\rho}|u\rangle$ by using Eq. (S34),

$$\langle -u|\hat{\rho}|u\rangle = \int P(\alpha)\langle -u|\alpha\rangle\langle\alpha|u\rangle \mathrm{d}^2\alpha. \tag{S36}$$

Substituting $\langle\alpha|u\rangle$ according to Eq. (S15), we obtain

$$\begin{aligned} \langle -u|\hat{\rho}|u\rangle &= \int P(\alpha) e^{-\frac{1}{2}|u|^2 - \frac{1}{2}|\alpha|^2 - u^*\alpha} e^{-\frac{1}{2}|u|^2 - \frac{1}{2}|\alpha|^2 + \alpha^* u}\, \mathrm{d}^2\alpha \\ &= e^{-|u|^2} \int P(\alpha) e^{-|\alpha|^2} e^{\alpha^* u - u^* \alpha}\, \mathrm{d}^2\alpha. \end{aligned} \tag{S37}$$

Introducing the variable substitution $\alpha = x + iy$ and $u = x' + iy'$, we obtain

$$\begin{aligned} \langle -u(x',y')|\hat{\rho}|u(x',y')\rangle e^{|u(x',y')|^2} &= \int P(\alpha(x,y)) e^{-x^2-y^2} e^{(x-iy)(x'+iy')-(x'-iy')(x+iy)}\, \mathrm{d}x\mathrm{d}y \\ &= \int P(\alpha(x,y)) e^{-x^2-y^2} e^{-i2yx'+i2y'x}\, \mathrm{d}x\mathrm{d}y. \end{aligned} \tag{S38}$$

Introducing the function $I(\tilde{x},\tilde{y})$ by

$$\begin{aligned} I(\tilde{x},\tilde{y}) &= \frac{1}{\pi^2}\int e^{i2x'\tilde{y}-i2y'\tilde{x}}\langle -u(x',y')|\hat{\rho}|u(x',y')\rangle e^{|u(x',y')|^2}\,\mathrm{d}x'\mathrm{d}y' \\ &= \frac{1}{\pi^2}\int P(\alpha(x,y))e^{-x^2-y^2}\int e^{-i2(y-\tilde{y})x'+iy'2(x-\tilde{x})}\,\mathrm{d}x'\mathrm{d}y'\,\mathrm{d}x\mathrm{d}y \\ &= \frac{1}{(2\pi)^2}\int P(\alpha(x,y))e^{-x^2-y^2}\int e^{-i(y-\tilde{y})x''+iy''(x-\tilde{x})}\,\mathrm{d}x''\mathrm{d}y''\,\mathrm{d}x\mathrm{d}y \\ &= \int P(\alpha(x,y))e^{-x^2-y^2}\delta(y-\tilde{y})\delta(x-\tilde{x})\,\mathrm{d}x\mathrm{d}y, \end{aligned} \tag{S39}$$

we conclude that

$$I(\tilde{x},\tilde{y}) = P(\alpha(\tilde{x},\tilde{y}))e^{-\tilde{x}^2-\tilde{y}^2}, \tag{S40}$$

which gives us

$$\begin{aligned} P(\alpha(x,y)) &= \frac{e^{x^2+y^2}}{\pi^2}\int e^{ix'y-iy'x}\langle -u(x',y')|\hat{\rho}|u(x',y')\rangle e^{|u(x',y')|^2}\,\mathrm{d}x'\mathrm{d}y', \\ P(\alpha) &= \frac{e^{|\alpha|^2}}{\pi^2}\int e^{-\alpha^* u+u^*\alpha}\langle -u|\hat{\rho}|u\rangle e^{|u|^2}\,\mathrm{d}^2u. \end{aligned} \tag{S41}$$

Pure coherent states. For the pure state $\hat{\rho}=|\beta\rangle\langle\beta|$, we obtain according to Eq. (S15)

$$\begin{aligned} \langle -u|\hat{\rho}|u\rangle &= e^{-\frac{1}{2}|-u-\beta|^2}e^{\frac{1}{2}(-u^*\beta+u\beta^*)}e^{-\frac{1}{2}|\beta-u|^2}e^{\frac{1}{2}(\beta^*u-\beta u^*)} \\ &= e^{-|u|^2}e^{-|\beta|^2}e^{u\beta^*-u^*\beta}. \end{aligned} \tag{S42}$$

Therefore, substituting Eq. (S42) into Eq. (S41), we obtain

$$\begin{aligned} P(\alpha) &= \frac{e^{|\alpha|^2}}{\pi^2}\int e^{-\alpha^*u+u^*\alpha}e^{-|u|^2}e^{-|\beta|^2}e^{u\beta^*-u^*\beta}e^{|u|^2}\,\mathrm{d}^2u \\ &= \frac{e^{|\alpha|^2}e^{-|\beta|^2}}{\pi^2}\int e^{-\alpha^*u+u^*\alpha}e^{u\beta^*-u^*\beta}\,\mathrm{d}^2u \\ &= \frac{e^{|\alpha|^2}e^{-|\beta|^2}}{\pi^2}\int e^{-u(\alpha-\beta)^*+u^*(\alpha-\beta)}\,\mathrm{d}^2u, \end{aligned} \tag{S43}$$

and considering that $u = x' + iy'$, we obtain

$$
\begin{aligned}
P(\alpha) &= \frac{e^{|\alpha|^2} e^{-|\beta|^2}}{\pi^2} \int e^{i2x' \operatorname{Im}(\alpha-\beta) - i2y' \operatorname{Re}(\alpha-\beta)} \, \mathrm{d}x' \mathrm{d}y' \\
&= \frac{e^{|\alpha|^2} e^{-|\beta|^2}}{(2\pi)^2} \int e^{ix'' \operatorname{Im}(\alpha-\beta) - iy'' \operatorname{Re}(\alpha-\beta)} \, \mathrm{d}x'' \mathrm{d}y'' \\
&= e^{|\alpha|^2} e^{-|\beta|^2} \delta(\operatorname{Im}(\alpha-\beta)) \delta(\operatorname{Re}(\alpha-\beta)) \\
&= \delta^2(\alpha-\beta).
\end{aligned}
\tag{S44}
$$

Hence, for a pure coherent state, $P(\alpha)$ coincides with the classical density of states. In particular, this shows that coherent states are classical-like quantum states.

Pure number states. The P-representation of a pure number state, $\hat{\rho} = |n\rangle\langle n|$, is obtained, as follows

$$
\begin{aligned}
\langle -u|\hat{\rho}|u\rangle &= \langle -u|n\rangle\langle n|u\rangle \\
&= e^{-|u|^2} \frac{u^n}{n!} (-u^*)^n,
\end{aligned}
\tag{S45}
$$

where we have substituted $\langle n|u\rangle$ in the second row, according to Eq. (S11), as follows

$$
\langle n|u\rangle = e^{-\frac{1}{2}|u|^2} \frac{u^n}{\sqrt{n!}}. \tag{S46}
$$

Therefore, substituting Eq. (S45) into Eq. (S41), we obtain

$$
\begin{aligned}
P(\alpha) &= \frac{e^{|\alpha|^2}}{\pi^2} \int e^{-\alpha^* u + u^* \alpha} \langle -u|\hat{\rho}|u\rangle e^{|u|^2} \, \mathrm{d}^2 u \\
&= \frac{e^{|\alpha|^2}}{\pi^2} \int e^{-\alpha^* u + u^* \alpha} e^{-|u|^2} \frac{(-uu^*)^n}{n!} e^{|u|^2} \, \mathrm{d}^2 u \\
&= \frac{e^{|\alpha|^2}}{n! \pi^2} \int e^{-\alpha^* u + u^* \alpha} (-uu^*)^n \, \mathrm{d}^2 u \\
&= \frac{e^{|\alpha|^2}}{n! \pi^2} \frac{\partial^{2n}}{\partial^n \alpha \partial^n \alpha^*} \int e^{-\alpha^* u + u^* \alpha} \, \mathrm{d}^2 u,
\end{aligned}
\tag{S47}
$$

which can also be written as

$$P(\alpha) = \frac{e^{|\alpha|^2}}{n!} \frac{\partial^{2n}}{\partial^n \alpha \partial^n \alpha^*} \delta^2 \alpha. \tag{S48}$$

Analogously, for an M-mode Gaussian state, we obtain

$$P_{\bigotimes_{j=1}^{M} |n_j\rangle\langle n_j|}(\alpha) = \prod_{j=1}^{M} \frac{e^{|\alpha_j|^2}}{n_j!} \frac{\partial^{2n_j}}{\partial^{n_j} \alpha_j \partial^{n_j} \alpha_j^*} \delta^2 \alpha_j. \tag{S49}$$

We note that this is the so-called *tempered distribution* function, which operates only as the argument of an integral, as follows

$$\int F(\alpha) \frac{\partial^{2n}}{\partial^n \alpha \partial^n \alpha^*} \delta^2 \alpha \, \mathrm{d}^2\alpha = \left. \frac{\partial^{2n} F(\alpha)}{\partial \alpha^n \partial^n \alpha^*} \right|_{\alpha=0,\, \alpha^*=0}. \tag{S50}$$

Expectation values for operators. In general, the P-representation of an operator $\hat{O}(\hat{a}^\dagger, \hat{a})$, is analogous to the representation of the density operator introduced by Eq. (S34). It involves the P-function $P_{\hat{O}}(\alpha)$, which is defined, as follows

$$\hat{O} = \int P_{\hat{O}}(\alpha) |\alpha\rangle\langle\alpha| \, \mathrm{d}^2\alpha, \tag{S51}$$

with expectation value given by

$$\begin{aligned} \langle \hat{O} \rangle &= \mathrm{Tr}[\hat{O}\hat{\rho}] \\ &= \sum_n \int P_{\hat{O}}(\alpha) \langle n|\alpha\rangle\langle\alpha|\hat{\rho}|n\rangle \, \mathrm{d}^2\alpha \\ &= \int P_{\hat{O}}(\alpha) \sum_n \langle\alpha|\hat{\rho}|n\rangle\langle n|\alpha\rangle \, \mathrm{d}^2\alpha \\ &= \int P_{\hat{O}}(\alpha) \langle\alpha|\hat{\rho}|\alpha\rangle \, \mathrm{d}^2\alpha \\ &= \pi \int P_{\hat{O}}(\alpha) Q(\alpha) \, \mathrm{d}^2\alpha, \end{aligned} \tag{S52}$$

where $Q(\alpha) = \pi^{-1}\langle\alpha|\hat{\rho}|\alpha\rangle$ is called the Husimi function. In particular, for a pure state $\hat{\rho} = |\psi\rangle\langle\psi|$, the Husimi function is $Q(\alpha) = \pi^{-1}|\langle\psi|\alpha\rangle|^2$. The derivation of the Husimi function for an multimode Gaussian will be the subject of the following subsection. For the particular case $\hat{O} = |n\rangle\langle n|$, we obtain:

$$\mathrm{Tr}[\hat{O}\hat{\rho}] = \mathrm{Tr}[\hat{\rho}|n\rangle\langle n|] = \pi \int P_{|n\rangle\langle n|}(\alpha) Q(\alpha)\, d^2\alpha, \tag{S53}$$

where $P_{|n\rangle\langle n|}(\alpha)$ is defined according to Eq. (S48) as

$$P_{|n\rangle\langle n|}(\alpha) = \frac{e^{|\alpha|^2}}{n!} \frac{\partial^{2n}}{\partial^n\alpha \partial^n\alpha^*} \delta^2\alpha, \tag{S54}$$

which yields

$$\mathrm{Tr}[\hat{\rho}|n\rangle\langle n|] = \pi \int Q(\alpha) \frac{e^{|\alpha|^2}}{n!} \frac{\partial^{2n}}{\partial^n\alpha \partial^n\alpha^*} \delta^2\alpha\, \mathrm{d}^2\alpha. \tag{S55}$$

1.3 Husimi function of an M-mode Gaussian state

The Husimi function of an M-mode Gaussian state is defined, as follows

$$Q(\alpha) = \pi^{-M}\langle\alpha|\hat{\rho}|\alpha\rangle, \tag{S56}$$

where $\alpha = (\alpha_1, \ldots, \alpha_M, \alpha_1^*, \ldots, \alpha_M^*)^T$. The goal of this subsection is to introduce the Wigner transform for the evaluation of Eq. (S56) for $M = 1$. As a result of this, we will obtain the following expression

$$Q(\alpha) = \frac{\pi^{-1}}{\sqrt{|\det(\sigma_Q)|}} e^{-\alpha^\dagger \sigma_Q^{-1} \alpha}, \tag{S57}$$

where $\sigma_Q = \sigma + I_2/2$.

Wigner transform. For the derivation of Eq. (S57), we first give the Husimi function for a single-mode pure Gaussian state. The elements of the density operator of a single-mode pure Gaussian state are given by

$$
\begin{aligned}
\langle x|\hat{\rho}|x'\rangle &= \langle x|\psi\rangle\langle\psi|x'\rangle \\
&= \left(\frac{\gamma}{\pi}\right)^{1/2} e^{-\frac{\gamma}{2}((x-d_x)^2+(x'-d_x)^2)+\frac{i}{\hbar}d_p(x-x')},
\end{aligned}
\tag{S58}
$$

where $d_x = \langle\hat{x}\rangle$, $d_p = \langle\hat{p}\rangle$, and $\gamma = (\langle(\hat{x}-d_x)^2\rangle)^{-1}/2$. These elements can be Wigner transformed, as follows

$$
\begin{aligned}
\rho_W(x,p) &= (2\pi\hbar)^{-1}\int e^{\frac{i}{\hbar}py}\left\langle x-\frac{y}{2}|\hat{\rho}|x+\frac{y}{2}\right\rangle \mathrm{d}y \\
&= (2\pi\hbar)^{-1}\int \left(\frac{\gamma}{\pi}\right)^{1/2} e^{-\frac{\gamma}{2}((x-\frac{y}{2}-d_x)^2+(x+\frac{y}{2}-d_x)^2)+\frac{i}{\hbar}(p-d_p)y}\,\mathrm{d}y \\
&= (2\pi\hbar)^{-1}e^{-\gamma(x^2-2xd_x+d_x^2)}\int \left(\frac{\gamma}{\pi}\right)^{1/2} e^{-\frac{\gamma}{4}y^2+\frac{i}{\hbar}(p-d_p)y}\,\mathrm{d}y \\
&= (\pi\hbar)^{-1}e^{-\left(\gamma(x-d_x)^2+(p-d_p)^2/(\hbar^2\gamma)\right)}.
\end{aligned}
\tag{S59}
$$

For a given positive constant $\gamma_\alpha > 0$, let $z = \left(\sqrt{\gamma_\alpha}(x-d_x), (p-d_p)/(\hbar\sqrt{\gamma_\alpha})\right)^T$, and

$$
\sigma = \begin{bmatrix} \gamma_\alpha/\gamma & 0 \\ 0 & \gamma/\gamma_\alpha \end{bmatrix}.
\tag{S60}
$$

We then obtain

$$
\begin{aligned}
\rho_W(x,p) &= \frac{e^{-z^T\sigma^{-1}z}}{\pi\hbar} \\
&= \frac{e^{-\frac{1}{2}z^T\tilde{\sigma}^{-1}z}}{2\pi\hbar\sqrt{|\det(\tilde{\sigma}|)}},
\end{aligned}
\tag{S61}
$$

where $\tilde{\sigma}^{-1} = 2\sigma^{-1}$.

Expectation values. Expectation values can be calculated in terms of the Wigner transform, as follows

$$\begin{aligned}\langle \hat{O} \rangle &= \mathrm{Tr}[\hat{\rho}\hat{O}] \\ &= \int \langle \tilde{x}|\hat{\rho}|\tilde{x}'\rangle\langle \tilde{x}'|\hat{O}|\tilde{x}\rangle \,\mathrm{d}\tilde{x}\mathrm{d}\tilde{x}' \\ &= \int \left\langle x - \frac{y}{2}|\hat{\rho}|x + \frac{y}{2}\right\rangle \left\langle x + \frac{y}{2}|\hat{O}|x - \frac{y}{2}\right\rangle \mathrm{d}x\mathrm{d}y,\end{aligned} \tag{S62}$$

where $\tilde{x} = x - \frac{y}{2}$ and $\tilde{x}' = x + \frac{y}{2}$. Therefore,

$$\begin{aligned}\langle \hat{O} \rangle &= \int \left\langle x - \frac{y}{2}|\hat{\rho}|x + \frac{y}{2}\right\rangle \int \left\langle x + \frac{y'}{2}|\hat{O}|x - \frac{y'}{2}\right\rangle \delta(y - y')\,\mathrm{d}y'\,\mathrm{d}x\mathrm{d}y \\ &= \frac{1}{2\pi\hbar}\int\int \left\langle x - \frac{y}{2}|\hat{\rho}|x + \frac{y}{2}\right\rangle e^{\frac{i}{\hbar}py} \int \left\langle x + \frac{y'}{2}|\hat{O}|x - \frac{y'}{2}\right\rangle e^{-\frac{i}{\hbar}py'}\,\mathrm{d}y'\,\mathrm{d}y\,\mathrm{d}x\mathrm{d}p \\ &= \int \rho_W(x,p) \int \left\langle x + \frac{y'}{2}|\hat{O}|x - \frac{y'}{2}\right\rangle e^{-\frac{i}{\hbar}py'}\,\mathrm{d}y'\,\mathrm{d}x\mathrm{d}p \\ &= \int \rho_W(x,p) \int \left\langle x - \frac{y'}{2}|\hat{O}|x + \frac{y'}{2}\right\rangle e^{\frac{i}{\hbar}py'}\,\mathrm{d}y'\,\mathrm{d}x\mathrm{d}p \\ &= \int \rho_W(x,p) O_W(x,p)\,\mathrm{d}x\mathrm{d}p,\end{aligned} \tag{S63}$$

where $O_W(x,p) = \int \left\langle x - \frac{y'}{2}|\hat{O}|x + \frac{y'}{2}\right\rangle e^{\frac{i}{\hbar}py'}\,\mathrm{d}y'$. In particular, the expectation value $\langle\alpha|\hat{\rho}|\alpha\rangle$ is given by

$$\langle\alpha|\hat{\rho}|\alpha\rangle = \int \rho_W(x,p) W_\alpha(x,p)\,\mathrm{d}x\mathrm{d}p, \tag{S64}$$

with $|\alpha\rangle$ defined according to Eq. (S32), and

$$\begin{aligned}W_\alpha(x,p) &= \int \left\langle x - \frac{y'}{2}|\alpha\right\rangle \left\langle \alpha|x + \frac{y'}{2}\right\rangle e^{\frac{i}{\hbar}py'}\,\mathrm{d}y' \\ &= 2e^{-\gamma_\alpha(x-q_\alpha)^2} e^{-(p-p_\alpha)^2/(\gamma_\alpha\hbar^2)},\end{aligned} \tag{S65}$$

with $\gamma_\alpha = m\omega/\hbar$, $q_\alpha = \langle\alpha|\hat{x}|\alpha\rangle$, and $p_\alpha = \langle\alpha|\hat{p}|\alpha\rangle$, corresponding to the value $\alpha = \sqrt{\gamma_\alpha/2}q_\alpha + i(2\gamma_\alpha)^{-1/2}\hbar^{-1}p_\alpha$, according to Eq. (S28). Analogously, we introduce $\beta =$

$\sqrt{\gamma_\alpha/2}x + i(2\gamma_\alpha)^{-1/2}\hbar^{-1}p$, from which we conclude that

$$2|\beta-\alpha|^2 = \gamma_\alpha(x-q_\alpha)^2 + (p-p_\alpha)^2/(\gamma_\alpha\hbar^2), \tag{S66}$$

which shows that

$$W_\alpha(x,p) = 2e^{-2|\beta-\alpha|^2}. \tag{S67}$$

Substituting Eqs. (S61) and (S67) into Eq. (S64), we find:

$$\begin{aligned}\langle\alpha|\hat{\rho}|\alpha\rangle &= \int \frac{e^{-\frac{1}{2}z^T\tilde{\sigma}^{-1}z}}{\pi\hbar\sqrt{|\det(\tilde{\sigma})|}}e^{-2|\beta-\alpha|^2}\,\mathrm{d}x\mathrm{d}p \\ &= \frac{1}{\pi\sqrt{|\det(\tilde{\sigma})|}}\int e^{-\frac{1}{2}\beta^\dagger\tilde{\sigma}^{-1}\beta}e^{-2|\beta-\alpha|^2}\,\mathrm{d}^2\beta.\end{aligned} \tag{S68}$$

For simplicity, let us consider the case where $d_x = d_p = 0$. Using that $|\beta-\alpha|^2 = (\beta-\alpha)^\dagger(\beta-\alpha) = \beta^\dagger\beta - \beta^\dagger\alpha - \alpha^\dagger\beta + \alpha^\dagger\alpha = \beta^\dagger\beta - 2\alpha^\dagger\beta + \alpha^\dagger\alpha$, we obtain

$$\begin{aligned}\langle\alpha|\hat{\rho}|\alpha\rangle &= \frac{e^{-2\alpha^\dagger\alpha}}{\pi\sqrt{|\det(\tilde{\sigma})|}}\int e^{-\frac{1}{2}\beta^\dagger(\tilde{\sigma}^{-1}+4)\beta}e^{4\alpha^\dagger\beta}\,\mathrm{d}^2\beta \\ &= \frac{2e^{-2\alpha^\dagger\alpha}}{\sqrt{|\det(\tilde{\sigma}^{-1}+4)||\det(\tilde{\sigma})|}}e^{\frac{1}{2}4\alpha^\dagger(\tilde{\sigma}^{-1}+4)^{-1}4\alpha} \\ &= \frac{2e^{-\alpha^\dagger(2-8(\tilde{\sigma}^{-1}+4)^{-1})\alpha}}{\sqrt{|\det(\tilde{\sigma}^{-1}+4)||\det(\tilde{\sigma})|}}.\end{aligned} \tag{S69}$$

Moreover, a short calculation shows that $2 - 8(\tilde{\sigma}^{-1}+4)^{-1} = (\sigma + I_2/2)^{-1}$, as well as $\sqrt{|\det(\tilde{\sigma}^{-1}+4)||\det(\tilde{\sigma})|} = 2\sqrt{|\det(I_2/2+\sigma)|}$. Therefore, we finally conclude that

$$\begin{aligned}Q(\alpha) &= \pi^{-1}\langle\alpha|\hat{\rho}|\alpha\rangle \\ &= \pi^{-1}\frac{e^{-\alpha^\dagger(\sigma+I_2/2)^{-1}\alpha}}{\sqrt{|\det(\sigma+I_2/2)|}},\end{aligned} \tag{S70}$$

which, when generalized to an M-mode Gaussian, gives Eq. (S57).

2 Output Probabilities of an M-mode Gaussian

In this section, we obtain the output probability distribution

$$\Pr(\bar{n}) = \mathrm{Tr}\left[\hat{\rho}\bigotimes_{j=1}^{M}|n_j\rangle\langle n_j|\right] \tag{S71}$$

for an M-mode input Gaussian, corresponding to occupation numbers of output modes $\bar{n}$ as described by the tensor product of number state operators $\hat{\bar{n}} = \bigotimes_{j=1}^{M}\hat{n}_j$, where $\hat{n}_j = |n_j\rangle\langle n_j|$ measures the probability of observing n_j photons in output mode j.

Substituting Eq. (S57) and Eq. (S54) into Eq. (S53), we obtain

$$\Pr(\bar{n}) = \int \frac{1}{\sqrt{|\det(\sigma_Q)|}} e^{-\frac{1}{2}\alpha^\dagger\sigma_Q^{-1}\alpha+\alpha^\dagger\alpha} \prod_{j=1}^{M}\frac{1}{n_j!}\frac{\partial^{2n_j}}{\partial^{n_j}\alpha_j\partial^{n_j}\alpha_j^*}\delta^2\alpha_j, \tag{S72}$$

and integration by parts yields

$$\Pr(\bar{n}) = \frac{1}{\sqrt{|\det(\sigma_Q)|}}\prod_{j=1}^{M}\frac{1}{n_j!}\frac{\partial^{2n_j}}{\partial^{n_j}\alpha_j\partial^{n_j}\alpha_j^*}e^{\frac{1}{2}\alpha^\dagger(I_{2M}-\sigma_Q^{-1})\alpha}\Bigg|_{\alpha_j=0}. \tag{S73}$$

We note that

$$\alpha^\dagger(I_{2M}-\sigma_Q^{-1})\alpha = \alpha^T\begin{bmatrix}0 & I_M\\ I_M & 0\end{bmatrix}(I_{2M}-\sigma_Q^{-1})\alpha, \tag{S74}$$

since is defined as $\alpha = (\alpha_1,\ldots,\alpha_M,\alpha_1^*,\ldots,\alpha_M^*)^T$. Hence,

$$\Pr(\bar{n}) = \frac{1}{\sqrt{|\det(\sigma_Q)|}}\prod_{j=1}^{M}\frac{1}{n_j!}\frac{\partial^{2n_j}}{\partial^{n_j}\alpha_j\partial^{n_j}\alpha_j^*}e^{\frac{1}{2}\alpha^T K\alpha}\Bigg|_{\alpha_j=0}, \tag{S75}$$

where we used

$$K = \begin{bmatrix} 0 & I_M \\ I_M & 0 \end{bmatrix} (I_{2M} - \sigma_Q^{-1}), \tag{S76}$$

as previously defined. In particular, for the specific case of measuring $n_j \in \{0, 1\}$ photons at each output mode, with $N = \sum_{j=1}^{M} n_j$, we obtain

$$\begin{aligned} \Pr(\bar{n}) &= \frac{1}{\sqrt{|\det(\sigma_Q)|}} \frac{\partial^{2N}}{\prod_{j=1}^{M} \partial^{n_j} \alpha_j \partial^{n_j} \alpha_j^*} e^{\frac{1}{2}\alpha^T K \alpha} \bigg|_{\alpha_j = 0} \\ &= \frac{1}{\sqrt{|\det \sigma_Q)|}} \frac{\partial^{2N}}{\prod_{l=1}^{N} \partial \alpha_l \partial \alpha_l^*} e^{\frac{1}{2}\alpha^T K \alpha} \bigg|_{\alpha_l = 0}, \end{aligned} \tag{S77}$$

where in the second row the indices $l = 1, \ldots, N$ correspond to the output modes with $n_j = 1$. To evaluate Eq. (S77), we introduce Faà di Bruno's formula in Sec. 3, showing that it can be evaluated, as follows

$$\begin{aligned} \Pr(\bar{n}) &= \frac{1}{\sqrt{|\det(\sigma_Q)|}} \sum_{j=1}^{(2N-1)!!} \prod_{k=1}^{N} K_{\mu_j(2k-1), \mu_j(2k)} \\ &= \frac{1}{\sqrt{|\det(\sigma_Q)|}} \mathrm{Haf}(K_S), \end{aligned} \tag{S78}$$

where $\mu_j \in S_{2N}$ (symmetric group of $2N$ elements) define the indices of measured photons (bright modes) corresponding to perfect matching j (of which there exist $(2N)!/(2^N N!) = (2N-1)!!$), and K_S is the submatrix of K corresponding to the indices of measured photons.

We observe that $\Pr(\bar{n})$ is directly proportional to the number of perfect matchings associated with the observed modes with indices $\bar{n}$ when A is the adjacency matrix of the complete graph of modes, $K = A^{\oplus 2} = c(A \oplus A)$, and K_S the submatrix of K corresponding to the observed modes. Therefore, the number of perfect matchings can be obtained by sampling from a Gaussian distribution with covariance $\sigma_Q = \sigma + I_{2M}/2$.

3 Faà di Bruno's formula

Equation (S75) can be evaluated as discussed by Kruse et al,[2] using Faà di Bruno's formula

$$\frac{\partial^n}{\partial x_1 \cdots \partial x_n} f(y) = \sum_{\pi \in P_n} f^{(|\pi|)}(y) \prod_{B \in \pi} \frac{\partial^{|B|} y}{\prod_{l \in B} \partial x_l}, \quad y = y(x_1, x_2, \ldots, x_n), \tag{S79}$$

where P_n is the set of partitions of n indices $\{1, 2, \ldots, n\}$, while $|\pi|$ is the number of blocks of partition π, and $|B|$ is the number of elements in block B.

Example 1. A simple example with $n = 3$ illustrates Eq. (S79) as applied to computing $\frac{\partial^3}{\partial x_1 \partial x_2 \partial x_3} f(y)$, with $y = y(x_1, x_2, x_3)$. The set P_3 of possible partitions of indices $\{1, 2, 3\}$ includes one partition π_1 with one block $\pi_1 = \{\{1, 2, 3\}\}$ ($|\pi_1| = 1$, one block of size three); three partitions with two blocks, including $\pi_2 = \{\{1, 2\}, \{3\}\}$, $\pi_3 = \{\{1, 3\}, \{2\}\}$, $\pi_4 = \{\{2, 3\}, \{1\}\}$ ($|\pi_{2,3,4}| = 2$); and finally one partition with three blocks $\pi_5 = \{\{1\}, \{2\}, \{3\}\}$ ($|\pi_5| = 3$). Hence, $|P_3| = 5$ and we obtain

$$\begin{aligned} \frac{\partial^3}{\partial x_1 \partial x_2 \partial x_3} f(y) = f'(y) \frac{\partial^3 y}{\partial x_1 \partial x_2 \partial x_3} + \ldots \\ f''(y) \left(\frac{\partial^2 y}{\partial x_1 \partial x_2} \frac{\partial y}{\partial x_3} + \frac{\partial^2 y}{\partial x_1 \partial x_3} \frac{\partial y}{\partial x_2} + \frac{\partial^2 y}{\partial x_2 \partial x_3} \frac{\partial y}{\partial x_1} \right) + \ldots \\ f'''(y) \frac{\partial y}{\partial x_1} \frac{\partial y}{\partial x_2} \frac{\partial y}{\partial x_3}. \end{aligned} \tag{S80}$$

Analogously, to evaluate Eq. (S77), we use $n = 2N$, $x = \alpha$, $y = \frac{1}{2}\alpha^T K \alpha$, and $f(y) = e^y$. Note that in this case $f^{(|\pi|)}(y) = f(y)$ for all partitions. It is important to note that the function $\frac{1}{2}\alpha^T K \alpha$ is quadratic in α, so all derivatives of third order or higher vanish. Furthermore, the argument of Eq. (S77) is evaluated at $\alpha_l = 0$, so all first order derivatives also vanish. This leaves only the partitions for which $|B| = 2$ for all blocks, which implies $|\pi| = N$ (*i.e.*, perfect matchings, the partitions of $2N$ indices into N blocks of pairs can be interpreted as permutations of the $2N$ photon indices). Therefore, we obtain

$$\frac{\partial^n}{\partial x_1 \cdots \partial x_n} f(y) = \frac{\partial^{2N} e^{\frac{1}{2}\alpha^T K \alpha}}{\prod_{l=1}^{N} \partial \alpha_l \partial \alpha_l^*} = e^{\frac{1}{2}\alpha^T K \alpha} \sum_{\pi \in PM} \prod_{B \in \pi} \frac{\partial^2 y}{\prod_{l \in B} \partial x_l}, \tag{S81}$$

where $PM \subset P_{2N}$ denotes the subset of perfect matchings. Using that the second-order derivatives of y can be expressed in terms of the matrix elements of K, we finally get

$$\begin{aligned} \Pr(\bar{n}) &= \frac{1}{\sqrt{|\det(\sigma_Q)|}} \frac{\partial^{2N}}{\prod_{l=1}^{N} \partial \alpha_l \partial \alpha_l^*} e^{\frac{1}{2}\alpha^T K \alpha} \Bigg|_{\alpha_l = 0} \\ &= \frac{1}{\sqrt{|\det(\sigma_Q)|}} \sum_{j=1}^{(2N-1)!!} \prod_{k=1}^{N} K_{\mu_j(2k-1), \mu_j(2k)} \\ &= \frac{1}{\sqrt{|\det(\sigma_Q)|}} \mathrm{Haf}(K_S), \end{aligned} \tag{S82}$$

Example 2. A simple example, with $N = 2$, shows how the partitions that contribute to Eq. (S81) can be interpreted as permutations of the photon indices. Let us assume that $M = 4$ and $N = 2$ photons are measured in the last two output modes 3 and 4. We then have $\alpha = \{\alpha_3, \alpha_4, \alpha_3^*, \alpha_4^*\}$. We label the indices as follows: $\{\alpha_3 \to 1, \alpha_4 \to 2, \alpha_3^* \to 3, \alpha_4^* \to 4\}$. The perfect matchings are given by

- $\pi_{PM_1} = \{\{1, 2\}, \{3, 4\}\}$
- $\pi_{PM_2} = \{\{1, 3\}, \{2, 4\}\}$
- $\pi_{PM_3} = \{\{1, 4\}, \{2, 3\}\}$

We therefore conclude that

$$\begin{aligned} \sum_{\pi \in PM} \prod_{B \in \pi} \frac{\partial^2 y}{\prod_{l \in B} \partial x_l} &= y_{1,2}^{(2)} y_{3,4}^{(2)} + y_{1,3}^{(2)} y_{2,4}^{(2)} + y_{1,4}^{(2)} y_{2,3}^{(2)} \\ &= \frac{\partial^2 y}{\partial \alpha_3 \partial \alpha_4} \frac{\partial^2 y}{\partial \alpha_3^* \partial \alpha_4^*} + \frac{\partial^2 y}{\partial \alpha_3 \partial \alpha_3^*} \frac{\partial^2 y}{\partial \alpha_4 \partial \alpha_4^*} + \frac{\partial^2 y}{\partial \alpha_3 \partial \alpha_4^*} \frac{\partial^2 y}{\partial \alpha_4 \partial \alpha_3^*} \\ &= K_{3,4} K_{7,8} + K_{3,7} K_{4,8} + K_{3,8} K_{4,7}. \end{aligned} \tag{S83}$$

We note that the index combinations of the partial derivatives in the first row can be mapped into permutations corresponding to perfect matchings. These permutations (Fig. S1) can be written in vector format as $\mu_1 = (1, 2, 3, 4)$, $\mu_2 = (1, 3, 2, 4)$ and $\mu_3 = (1, 4, 2, 3)$, also denoted as $\sigma_1 = \text{id}$, $\sigma_2 = (23)$, and $\sigma_3 = (243)$. Note, that the blocks are ordered from left to right corresponding to their block indices from lowest to highest and the numbers within a block are also in increasing order, so $\mu_j(2k-1) < \mu_j(2k+1)$ and $\mu_j(2k-1) < \mu_j(2k)$.

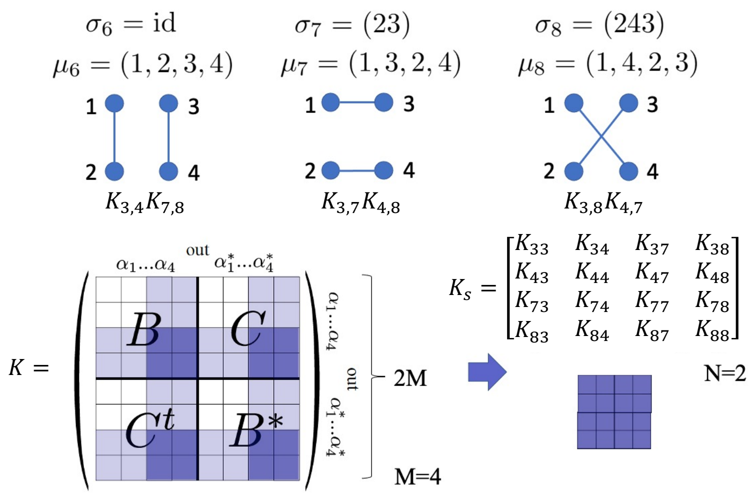

Figure S1: Top: Index combinations as perfect matchings of a graph with four nodes. Bottom: Construction of the 2×2 submatrix K_S from the 8×8 symmetric matrix $K = A^{\oplus 2}$ for two photons measured in the last two output modes 3 and 4.

4 Covariance matrix of squeezed and rotated state

The goal of Appendices 4 and 5 is to prove Eq. 13 in the main text, which establishes a relationship between the covariance matrix of the M-mode squeezed and rotated state, σ, and the graph adjacency matrix A. In this appendix, we first give the expression of σ expressed according to the squeezing parameters and the M-mode rotation matrix $\mathbf{U}$ that defines the linear interferometer. Then in Appendix 5 we show how $A^{\oplus 2} = cA \oplus cA$ is identified as the so-called kernel matrix K, which one-to-one correspond to the covariance matrix σ.

Recall the definition of the squeezing operation

$$\hat{S}(r) = e^{(-r(\hat{a})^2 + r(\hat{a}^\dagger)^2)/2}, \tag{S84}$$

where the real-valued r is referred to as the squeezing parameter. We aim to show that the action of the squeezing operator on the creation and annihilation operators are equivalent to the following linear Bogoliubov transformation

$$\begin{bmatrix} \hat{a} \\ \hat{a}^\dagger \end{bmatrix} \mapsto \begin{bmatrix} \cosh(r) & \sinh(r) \\ \sinh(r) & \cosh(r) \end{bmatrix} \begin{bmatrix} \hat{a} \\ \hat{a}^\dagger \end{bmatrix} = \begin{bmatrix} \hat{a}' \\ (\hat{a}')^\dagger \end{bmatrix}. \tag{S85}$$

To proof this relationship, we derive the following

$$\hat{S}(r)^\dagger \hat{a} \hat{S}(r) = \cosh(r)\hat{a} + \sinh(r)\hat{a}^\dagger. \tag{S86}$$

We set

$$\hat{A} = (r(\hat{a})^2 - r(\hat{a}^\dagger)^2)/2, \tag{S87}$$

so that $\hat{S}(r)^\dagger = e^{\hat{A}}$. Then, using the Baker–Campbell–Hausdorff formula, we have

$$\begin{aligned} \hat{S}(r)^\dagger \hat{a} \hat{S}(r) &= e^{\hat{A}} \hat{a} e^{-\hat{A}} \\ &= \sum_{k=0}^{\infty} \frac{1}{k!} [\hat{A}, [\hat{A}, \ldots [\hat{A}, \hat{a}] \ldots]], \end{aligned} \tag{S88}$$

where each term contains k commutators. Noting that

$$\begin{aligned} [\hat{A}, \hat{a}] &= \frac{1}{2}[r(\hat{a})^2 - r(\hat{a}^\dagger)^2, \hat{a}] = r\hat{a}^\dagger, \\ [\hat{A}, \hat{a}^\dagger] &= r\hat{a}, \end{aligned} \tag{S89}$$

we have

$$[\hat{A}, \dots [\hat{A}, \hat{a}] \dots]] = \begin{cases} r^k \hat{a} & \text{if } k \text{ is even,} \\ r^k \hat{a}^\dagger & \text{if } k \text{ is odd.} \end{cases} \tag{S90}$$

Then we obtain

$$\begin{aligned} \hat{S}(r)^\dagger \hat{a} \hat{S}(r) &= \hat{a} \sum_{k=0}^{\infty} \frac{r^{2k}}{(2k)!} + \hat{a}^\dagger \sum_{k=0}^{\infty} \frac{r^{2k+1}}{(2k+1)!} \\ &= \hat{a}\mathrm{cosh}(r) + \hat{a}^\dagger \mathrm{sinh}(r). \end{aligned} \tag{S91}$$

We now show that the covariance matrix of single mode squeezed state is

$$\sigma'(r) = \frac{1}{2} \begin{bmatrix} \cosh^2(r) + \sinh^2(r) & 2\mathrm{cosh}(r)\mathrm{sinh}(r) \\ 2\mathrm{cosh}(r)\mathrm{sinh}(r) & \cosh^2(r) + \sinh^2(r) \end{bmatrix}. \tag{S92}$$

For the first element of the squeezed state covariance matrix σ'_{11}, we substitute in the definition of the covariance matrix in Eq. 3 in the main text

$$\begin{aligned} \sigma'_{11} &= \frac{1}{2} \langle \{ \hat{a}', (\hat{a}')^\dagger \} \rangle \\ &= \frac{1}{2} \langle \hat{a}' (\hat{a}')^\dagger + (\hat{a}')^\dagger \hat{a}' \rangle \\ &= \frac{1}{2} \langle (\mathrm{cosh}(r)^2 + \mathrm{sinh}(r)^2)(\hat{a}\hat{a}^\dagger + \hat{a}^\dagger \hat{a}) + 2\mathrm{sinh}(r)\mathrm{cosh}(r)(\hat{a}\hat{a} + \hat{a}^\dagger \hat{a}^\dagger) \rangle \\ &= \frac{1}{2} (\mathrm{cosh}(r)^2 + \mathrm{sinh}(r)^2) \langle \hat{a}\hat{a}^\dagger + \hat{a}^\dagger \hat{a} \rangle + \mathrm{sinh}(r)\mathrm{cosh}(r) \langle (\hat{a}\hat{a} + \hat{a}^\dagger \hat{a}^\dagger) \rangle \\ &= \frac{1}{2} (\mathrm{cosh}(r)^2 + \mathrm{sinh}(r)^2), \end{aligned} \tag{S93}$$

where the last equality uses $\langle \hat{a}\hat{a}^\dagger + \hat{a}^\dagger \hat{a} \rangle = 1$ and $\langle \hat{a}\hat{a} \rangle = \langle \hat{a}^\dagger \hat{a}^\dagger \rangle = 0$ for the vacuum state. Note that all averages are taken for the vacuum state density matrix since the creation and annihilation operators are in the Heisenberg representation. Similarly,

$$\begin{aligned}
\sigma'_{12} &= \frac{1}{2}\langle 2\hat{a}'\hat{a}'\rangle \\
&= \langle(\cosh(r)\hat{a} + \sinh(r)\hat{a}^\dagger)(\cosh(r)\hat{a} + \sinh(r)\hat{a}^\dagger)\rangle \\
&= \langle\cosh(r)^2(\hat{a}\hat{a}) + \sinh(r)^2(\hat{a}^\dagger\hat{a}^\dagger) + 2\sinh(r)\cosh(r)\{\hat{a}^\dagger, \hat{a}\}\rangle \\
&= \sinh(r)\cosh(r).
\end{aligned} \tag{S94}$$

The derivation for the other two elements of σ' are analogous. Gathering all elements we obtain Eq. (S92).

Next, we show that applying an M-mode rotation, specified by an $M \times M$ unitary rotation matrix U, on the single-mode squeezed states specified by Eq. (S92), results in a state with the following covariance matrix

$$\sigma = \begin{bmatrix} U & 0 \\ 0 & U^* \end{bmatrix} \sigma_{\text{sque}} \begin{bmatrix} U^* & 0 \\ 0 & U \end{bmatrix}^T, \tag{S95}$$

where σ_{sque} is the generalization of Eq. (S92) to M modes, as shown in Eq. 24 in the main text. To prove this, we first write a given $2M \times 2M$ covariance matrix $\tilde{\sigma}$ in the following block form

$$\tilde{\sigma} = \begin{bmatrix} B & G \\ D & C \end{bmatrix}, \tag{S96}$$

where all four blocks are $M \times M$ matrices. We now show that an M-mode rotation specified by the $M \times M$ unitary matrix U would rotate the covariance matrix to be

$$\tilde{\sigma}' = \begin{bmatrix} U & 0 \\ 0 & U^* \end{bmatrix} \tilde{\sigma} \begin{bmatrix} U^* & 0 \\ 0 & U \end{bmatrix}^T = \begin{bmatrix} B' & G' \\ D' & C' \end{bmatrix}, \tag{S97}$$

where $B^{'} = UBU^{\dagger}$, $C^{'} = U^{*}CU^{T}$, $G^{'} = UGU^{T}$, $D^{'} = U^{*}DU^{\dagger}$. As derived in Eq. 28 in the main text, the M-mode rotation linearly combines all M original annihilation/creation operators to obtain the rotated annihilation/creation operators, with the combination coefficients specified by elements of U

$$\begin{aligned} \hat{a}_k^{'} &= \sum_{j=1}^{M} U_{kj}\hat{a}_j, \\ (\hat{a}_k^{'})^{\dagger} &= \sum_{j=1}^{M} U_{kj}^{*}\hat{a}_j^{\dagger}. \end{aligned} \tag{S98}$$

According to the definition of the covariance matrix in Eq. 3 in the main text, an element $\sigma_{ij}^{'}$ of the upper-left block B $(1 \leq i, j \leq M)$ of the rotated covariance matrix $\sigma^{'}$, can be expanded as

$$\begin{aligned} \tilde{\sigma}_{ij}^{'} &= \left\langle \{\hat{a}_i^{'}(\hat{a}_j^{'})^{\dagger}\} \right\rangle /2 \\ &= \left\langle \hat{a}_i^{'}(\hat{a}_j^{'})^{\dagger} + (\hat{a}_j^{'})^{\dagger}\hat{a}_i^{'} \right\rangle /2 \\ &= \frac{1}{2}\left\langle \left(\sum_{l=1}^{M} U_{il}\hat{a}_l\right)\left(\sum_{m=1}^{M} U_{jm}^{*}\hat{a}_m^{\dagger}\right) + \left(\sum_{m=1}^{M} U_{jm}^{*}\hat{a}_m^{\dagger}\right)\left(\sum_{l=1}^{M} U_{il}\hat{a}_l\right) \right\rangle \\ &= \frac{1}{2}\sum_{l,m=1}^{M} U_{il}U_{jm}^{*}\left\langle \hat{a}_l\hat{a}_m^{\dagger} + \hat{a}_m^{\dagger}\hat{a}_l \right\rangle \\ &= \sum_{l,m=1}^{M} U_{il}\tilde{\sigma}_{lm}U_{mj}^{\dagger} \\ &= (UBU^{\dagger})_{ij}, \end{aligned} \tag{S99}$$

which proves $B^{'} = UBU^{\dagger}$. The same procedure is carried out for C, G and D to prove Eq. (S97). In particular, with $\tilde{\sigma} = \sigma_{\text{sque}}$, we have

$$\sigma_{\text{out}} = \begin{bmatrix} U & 0 \\ 0 & U^{*} \end{bmatrix} \sigma_{\text{sque}} \begin{bmatrix} U^{*} & 0 \\ 0 & U \end{bmatrix}^{T}, \tag{S100}$$

as in Eq. 30 in the main text.

5 Kernel matrix for the N-mode rotated state

The goal of this section is to prove Eq. 13 in the main text. First, we show that the squeezed state covariance matrix $\sigma'(r)$, derived as in Eq. (S92), corresponds to the kernel matrix $K(r)$ that has the following form

$$K(r) = \begin{bmatrix} \tanh(r) & 0 \\ 0 & \tanh(r) \end{bmatrix}, \tag{S101}$$

where the kernel matrix K of a Gaussian state is defined according to its covariance matrix:

$$\begin{aligned} \sigma_Q &= \sigma + I/2, \\ K &= X(I - \sigma_Q^{-1}), \\ X &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \end{aligned} \tag{S102}$$

According to Eqs. (S92) and (S102),

$$\begin{aligned} \sigma'_Q(r) &= \sigma'(r) + I/2 \\ &= \frac{1}{2}\begin{bmatrix} \cosh^2(r) + \sinh^2(r) + 1 & 2\cosh(r)\sinh(r) \\ 2\cosh(r)\sinh(r) & \cosh^2(r) + \sinh^2(r) + 1 \end{bmatrix} \\ &= \begin{bmatrix} \cosh^2(r) & \cosh(r)\sinh(r) \\ \cosh(r)\sinh(r) & \cosh^2(r) \end{bmatrix}. \end{aligned} \tag{S103}$$

Taking the inverse of the matrix,

$$
\begin{aligned}
(\sigma'_Q(r))^{-1} &= \frac{1}{\cosh^4(r) - \sinh^2(r)\cosh^2(r)} \begin{bmatrix} \cosh^2(r) & -\cosh(r)\sinh(r) \\ -\cosh(r)\sinh(r) & \cosh^2(r) \end{bmatrix} \\
&= \frac{1}{\cosh^2(r)} \begin{bmatrix} \cosh^2(r) & -\cosh(r)\sinh(r) \\ -\cosh(r)\sinh(r) & \cosh^2(r) \end{bmatrix} \\
&= \begin{bmatrix} 1 & -\tanh(r) \\ -\tanh(r) & 1 \end{bmatrix},
\end{aligned} \tag{S104}
$$

and substitution in the definition for K yields

$$
\begin{aligned}
K(r) &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \left(\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \begin{bmatrix} 1 & -\tanh(r) \\ -\tanh(r) & 1 \end{bmatrix} \right) \\
&= \begin{bmatrix} \tanh(r) & 0 \\ 0 & \tanh(r) \end{bmatrix}.
\end{aligned} \tag{S105}
$$

The results above are for 1-mode squeezed states. Generalizing to M-single-mode squeezed states is trivial since all modes are unentangled with each other. In that case, we have

$$
I_M - \sigma^{-1}_{M-squeezed,Q} = \begin{bmatrix} 0 & \bigoplus_{j=1}^{M} \tanh(r_j) \\ \bigoplus_{j=1}^{M} \tanh(r_j) & 0 \end{bmatrix} \tag{S106}
$$

$$
, \tag{S107}
$$

and the M-mode squeezed state kernel matrix is

$$
K_{M-squeezed} = \begin{bmatrix} \bigoplus_{j=1}^{M} \tanh(r_j) & 0 \\ 0 & \bigoplus_{j=1}^{M} \tanh(r_j) \end{bmatrix}. \tag{S108}
$$

Now we show that the covariance matrix of the N-mode squeezed state in Eq. (S100) corresponds to the following kernel matrix

$$K = c(A \oplus A) =: A^{\oplus 2}, \tag{S109}$$

where the adjacency matrix A is decomposed according to Takagi's factorization as

$$A = U \left(\frac{1}{c} \bigoplus_{j=1}^{M} \tanh(r_j) \right) U^T, \tag{S110}$$

where $1/c$ is a constant greater than the largest singular value of A, ensuring that every scaled singular value can be represented by the form of $\tanh(r_j)$. We begin by setting

$$\tilde{U} = \begin{bmatrix} U & 0 \\ 0 & U^* \end{bmatrix}, \tag{S111}$$

so that Eq. (S100) becomes

$$\sigma = \tilde{U}\sigma'(r)\tilde{U}^\dagger. \tag{S112}$$

The corresponding matrix $\sigma_Q = \sigma + I/2$ can be written as

$$\begin{aligned} \sigma_Q &= \sigma + I/2 \\ &= \tilde{U}\sigma'(r)\tilde{U}^\dagger + \tilde{U}I\tilde{U}^\dagger/2 \\ &= \tilde{U}\left(\sigma'(r) + I/2\right)\tilde{U}^\dagger \\ &= \tilde{U}\sigma'_Q(r)\tilde{U}^\dagger. \end{aligned} \tag{S113}$$

Moreover, since $\tilde{U}$ is unitary,

$$\sigma_Q^{-1} = \tilde{U}\sigma'_Q(r)^{-1}\tilde{U}^\dagger. \tag{S114}$$

Therefore,

$$
\begin{aligned}
I-\sigma_Q^{-1} &= I-\tilde{U}\sigma_Q'(r)^{-1}\tilde{U}^\dagger \\
&= \tilde{U}\left(I-\sigma_Q'(r)^{-1}\right)\tilde{U}^\dagger \\
&= \tilde{U}\begin{bmatrix} 0 & \bigoplus_{j=1}^N \tanh(r_j) \\ \bigoplus_{j=1}^N \tanh(r_j) & 0 \end{bmatrix}\tilde{U}^\dagger \\
&= \begin{bmatrix} U & 0 \\ 0 & U^* \end{bmatrix}\begin{bmatrix} 0 & \bigoplus_{j=1}^N \tanh(r_j) \\ \bigoplus_{j=1}^N \tanh(r_j) & 0 \end{bmatrix}\begin{bmatrix} U^\dagger & 0 \\ 0 & U^T \end{bmatrix} \\
&= \begin{bmatrix} 0 & U\bigoplus_{j=1}^N \tanh(r_j)U^T \\ U^*\bigoplus_{j=1}^N \tanh(r_j)U^\dagger & 0 \end{bmatrix},
\end{aligned} \tag{S115}
$$

where the third equality is obtained according to Eq. (S106). The kernel matrix $K = X_{2M}\left(I_{2M}-\sigma_Q^{-1}\right)$ is then

$$
\begin{aligned}
K &= \begin{bmatrix} 0 & I_M \\ I_M & 0 \end{bmatrix}\begin{bmatrix} 0 & U\bigoplus_{j=1}^M \tanh(r_j)U^T \\ U^*\bigoplus_{j}^M \tanh(r_j)U^\dagger & 0 \end{bmatrix} \\
&= \begin{bmatrix} U^*\bigoplus_{j=1}^M \tanh(r_j)U^\dagger & 0 \\ 0 & U\bigoplus_{j=1}^M \tanh(r_j)U^T \end{bmatrix} \\
&= cA^*\oplus cA \\
&= c(A\oplus A) \\
&= A^{\oplus 2},
\end{aligned} \tag{S116}
$$

since A is real.

References

(1) Kais, S.; Levine, R. D. Coherent states for the Morse oscillator. *Physical Review A* **1990**, *41*, 2301–2305.

(2) Kruse, R.; Hamilton, C. S.; Sansoni, L.; Barkhofen, S.; Silberhorn, C.; Jex, I. Detailed study of Gaussian boson sampling. *Phys. Rev. A* **2019**, *100*, 032326.