Non-classicality of bosonic fields in states of undefined particle numbers

A thesis presented for the degree of Doctor of Philosophy

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STRESZCZENIE

Odkrycie odmiennego od klasycznego zachowania układów składających się z małej ilości cząstek sprowokowało wiele fundamentalnych pytań o naturę naszego świata. Dalszy rozwój mechaniki kwantowej otworzył również nowe perspektywy na wykorzystanie zjawisk kwantowych w kontekście nowych technologii. W związku z tym, badanie zjawisk nieklasycznych stało się jednym z głównych nurtów badań w dziedzinie fizyki. Wraz z coraz większym zrozumieniem prostych układów zawierających niewielką liczbę cząstek, problematyka układów bardziej złożonych staje się przedmiotem zainteresowania zarówno z punktu widzenia złożonych zastosowań, jak i fundamentalnego pytania kiedy efekty kwantowe pozostają istotne. Motywuje to rozważania nad układami zawierającymi nieokreśloną liczbę cząstek, w których cechy kwantowe nadal odgrywają ważną rolę.

Niniejsza rozprawa doktorska jest podsumowaniem serii prac współautorstwa doktoranta, skoncentrowanych na opisie zjawisk nieklasycznych w układach bozonowych zawierających nieokreśloną liczbę cząstek, zwłaszcza w reżimie dużej średniej liczby cząstek.

W pierwszym artykule zatytułowanym "Simplified quantum optical Stokes observables and Bell's theorem" zostały opisane nowe obserwable, które pozwalają na wykrycie nieklasyczności Bella, korzystając z polaryzacyjnych stanów splątanych o nieokreślonej liczbie fotonów. Co istotne zaproponowany pomiar umożliwia wykrycie nieklasyczności w zakresie średniej liczby fotonów znacznie przekraczającej inne dotychczasowe podejścia. Zaproponowane obserwable przypisują jako wynik pomiaru ± 1 bądź 0 w zależności od znaku zmierzonej różnicy odpowiedzi detektorów wykrywających fotony w dwóch ortogonalnych modach polaryzacji. W związku z tym obsrwable te można zrealizować za pomocą dowolnego typu detektorów natężenia światła, dla których odpowiedź detektorów rośnie wraz z liczbą fotonów.

Drugi artykuł "Bosonic fields in states with undefined particle numbers possess detectable non-contextuality features, plus more" przedstawia nową reprezentację algebry $\mathfrak{su}(2)$ na dwumodowej bozonowej przestrzeni Focka. Otrzymany zestaw operatorów pozwolił na zaproponowanie uogólnionego kwadratu Peresa-Mermina, a tym samym na opis nieklasycznego efektu kontekstualności dla pól bozonowych o nieokreślonej liczbie cząstek. Co więcej, efekt ten jest powszechny dla stanów o dużej liczbie cząstek, osiągając dla przyjętego kryterium ograniczenie kwantowe w granicach makroskopowej średniej liczby cząstek. Takie zachowanie jest nietypowe dla rozważań zjawisk kwantowych.

Trzeci artykuł z serii "Generalization of Gisin's Theorem to Quantum Fields" dotyczy sformułowania twierdzenia Gisina w kontekście pól kwantowych. Przedstawione uogólnienie tego twierdzenia stwierdza, że każdy czysty stan splątany pola kwantowego narusza pewną nierówność Bella. Wobec tego nieklasyczność Bella w ramach kwantowej teorii pola jest obecna dla wszystkich stanów czystych układów splątanych, nawet jeśli liczba cząstek jest nieokreślona;

Ostatnia praca zatytułowana "Open dynamics of entanglement in mesoscopic bosonic systems" wprowadza nowy mezoskopowy opis pól bozonowych, który pozwala na rozważenie otwartej ewolucji splątania. Opisy mezoskopowe mają na celu uproszczenie różnych problemów poprzez uwzględnienie tylko najważniejszych stopni swobody. Zaproponowany opis opiera się w szczególności na korelacjach w liczbie cząstek. Na podstawie tych korelacji skonstruowane zostało rozszerzenie zaproponowanego niedawno formalizmu zredukowanego pola, który jednak sam w sobie nie zawiera informacji o splątaniu. Zaprezentowany formalizm matematycznie odzwierciedla przestrzeń Hilberta dwóch cząstek w ramach pierwszej kwantyzacji i dlatego pozwala na intuicyjne wykorzystanie znanych już narzędzi mechaniki kwantowej. W pracy pokazane zostało, że zaproponowany formalizm jest w stanie opisać splątanie zarówno stanów gaussowskich, jak i niegaussowskich. Ponadto formalizm ten nie ogranicza się tylko do opisu splątania. W ramach przykładu zaprezentowane zostało jak nieklasyczny efekt statystyki sub-Poissonowskiej przekształca się w splątanie poprzez działanie rozdzielacza wiązki.

ABSTRACT

The discovery of the quantum behavior of small-scale systems resulted in a plethora of fundamental questions about the nature of our world. It also provided new avenues for the development of technologies that utilize quantum phenomena. Therefore, the study of non-classical phenomena became one of the core subjects in physics. With an increasing understanding of simple systems containing a small and fixed number of particles, the problems of more complex systems gain increasing attention, both from the point of view of more complex applications and the fundamental question of when quantum effects play an important role. This motivates studies of quantum fields in states of undefined particle numbers in which quantum features still play an important role.

This PhD dissertation summarizes a series of papers, coauthored by the PhD candidate, concentrated on describing non-classical phenomena in bosonic systems containing an undefined number of particles, especially in the regime of high average numbers of particles.

The first article "Simplified quantum optical Stokes observables and Bell's theorem" describes new observables that allow for the detection of Bell non-classicality of polarization-entangled states with an undefined number of photons. In particular, the proposed measurement scheme enables detection of non-classicality in the range of average number of photons that greatly exceeds previous approaches. These observables can be realized with any intensity measurement for which the response of the apparatus increases with the number of photons. This is because they are constructed as a sign of the difference in the response of the detectors detecting photons in two orthogonal polarization modes.

The second article "Bosonic fields in states with undefined particle numbers possess detectable non-contextuality features, plus more" presents a new representation of $\mathfrak{su}(2)$ algebra on a two-mode bosonic Fock space. The resulting set of operators enabled us to propose a generalized Peres-Mermin square, and thus to describe non-classical effects of contextuality for bosonic fields with an undefined number of particles. What is more, the effect becomes a common feature of states with a high number of particles, reaching quantum bounds for the used criterion in the limits of macroscopic average numbers of particles; a behavior which is rare in considerations of quantum phenomena.

The third article in the series "Generalization of Gisin's Theorem to Quantum Fields" concerns the problem of Gisin's theorem in the context of quantum fields. Our generalization states that any pure entangled state of a quantum field violates some Bell inequality. Thus, Bell non-classicality within the framework of quantum field theory is present in pure states of all entangled systems even when the number of particles is undefined;

The last paper "Open dynamics of entanglement in mesoscopic bosonic systems" proposes a mesoscopic description of bosonic fields that allows considerations of the open evolution of discrete variable entanglement. Mesoscopic descriptions aim to simplify different problems by considering only the most important degrees of freedom. The proposed description is based on the correlations in particle numbers. With these correlations, we build the extension of the recently proposed reduced state of the field formalism, which, however, by itself does not contain information about entanglement. Our formalism mathematically resembles the first quantization Hilbert space of two particles and therefore allows for the intuitive use of already known tools of quantum mechanics. We show that it is able to describe the entanglement of both Gaussian and non-Gaussian states. In addition, this formalism is not limited to describing entanglement. As an example for this, we consider how the non-classical effect of sub-Poissonian statistics is transformed into entanglement through the action of the beamsplitter.

I. INTRODUCTION

The appearance of the mathematical paradigm of quantum mechanics at the beginning of the twentieth century with its remarkable successes in providing an explanation to the multiple observations which could not be described within classical theory forced a sudden shift in the way we perceive our universe. The unintuitive probabilistic character of quantum mechanics posed fundamental questions about how we should interpret nature. This started a full-of-controversies ongoing debate on the interpretation of quantum mechanics. One of the milestones in understanding quantum physics started with the famous EPR paradox [1] based on a peculiar quantum phenomenon later called entanglement. The apparent conclusion of this paradox was the incompleteness of quantum mechanics. This reasoning was based on a strong belief inherited from classical mechanics about the determinism of the world and argued that the probabilistic nature of quantum mechanics emerges from our lack of knowledge about some underlying deterministic local hidden elements of reality. The following discourse in the physics community [2–4] long waited for the breakthrough in the form of Bell's Theorem [5] which stated that predictions of quantum mechanics are incompatible with any local hidden variable (LHV) model. Finally, experiments [6, 7] were conducted that followed the predictions of quantum mechanics rather than LHV models. This once and for all ended this debate and showed that the classical way of thinking solely in terms of deterministic local hidden variables is invalid.

A deeper understanding of the concept of superposition and entanglement had an impact not only on the fundamental understanding of physics but also enabled the application of these phenomena in multiple tasks. The appearance of the concept of the qubit, that is, a two-level system, the state of which can act as a classical bit but also expands its capabilities by maintaining quantum features, laid the foundation for the field of Quantum Information. One of the key avenues in this field is quantum computation, which promises a speed-up in computation tasks for which classical computers require enormous amounts of time. An example of such a task is the simulation of quantum systems such as molecules [8, 9]. Therefore, proper quantum simulators would allow for the easier development of new medicines and materials. The appearance of multiple algorithms for quantum computers that provide a speed-up, like the famous Shor's algorithm for factorization of integers [10] or Grover's search algorithm [11], made quantum computing one of the primary focus in physics research. At the same time, this increased interest in research on entanglement, as it underlies numerous quantum computing algorithms [12]. Another avenue in quantum information is quantum cryptography. It emerged with the proposition of the first quantum key distribution algorithm BB84 [13], in which the superposition of the state of the medium used for the distribution of secret key enables detecting eavesdropping. Further on, the Ekert91 algorithm [14], which is based on entanglement, resulted in the development of the most secure method of information sharing, i.e., device-independent quantum key distribution [15, 16]. This class of algorithms relies only on observed correlations without assumptions on the measurement device itself to provide uncompromised shared bits by utilizing the Bell test. This methodology is based on the fact that violation of Bell inequality ensures that appearing correlations cannot result from a LHV model, and therefore third parties cannot have deterministic knowledge about all the outcomes. As data security is one of the key areas for public security, one could expect entanglement to be at the center of broadly used technologies of the future.

A crucial problem is finding the best implementation of these new quantum devices. As in quantum cryptography, information has to be distributed over long distances, the answer is photonic systems [17–19]. While for quantum computation there are different viable options, photonic systems could be also utilized in this context. This is especially the case, as one can construct universal photonic quantum computers using simple linear optics [20]. In fact, there are different possible approaches in reaching universal quantum computing with photonic systems, for example, gate-based [21, 22], measurement-based [23, 24], and fusion-based [25]. Besides universal quantum computing, the more task-specific devices are of interest for presenting quantum advantage, as such devices could be easier to implement. For photonic systems, the highly studied example of such a task is boson sampling [26], which was shown to be a hard problem for a classical computer if the conjectured polynomial hierarchy for complexity classes holds. Therefore, despite the lack of known practical applications of such a task, it is pursued with the goal of experimental presentation of a quantum advantage. Photonic systems are also considered in the context of quantum machine learning using, e.g., quantum neural networks [27, 28] or quantum reservoir computing

[29, 30]. Recent developments in integrated photonics [31, 32] that allow production of on-chip devices are currently the most promising avenue for scaling quantum photonic devices. However, the bosonic nature of photonic modes complicates even the simplest systems, as each mode can be occupied by an undefined number of particles. Therefore, the implementation of qubits in photonic systems is approximate, as one can expect losses of photons that encode information and also noise coming from additional photons entering the system from the environment. One is also not confined to consideration of qubits in photonic modes, but one has infinite-dimensional state space to explore for non-classical effects. All of this adds complexity to the problem of detecting non-classical phenomena like entanglement. Still, multiple methods for observing the non-classicality of bosonic states have been introduced [33, 34].

In general, a major obstacle in the implementation of quantum hardware is the decoherence effects, which can easily appear in complex systems. This is especially true, as the goal of the system size required for real-life application of quantum computers still exceeds current technology by a few orders of magnitude, and one needs to prevent the disappearance of quantum effects in such systems for proper operation. What is more, minimization of the effects of decoherence, for example, using decoherence-free subspaces [35], is also crucial in quantum cryptography to increase the range at which one can perform communication schemes. The increasing complexity of the systems also casts a full quantum description of such systems infeasible. Therefore, one of the important research subjects is the development of simpler descriptions of such systems that maintain the most important quantum features of the system. Thus, the goal of such mesoscopic descriptions is to allow for a theoretical analysis of complex systems, which could be found useful further in designing hardware.

The description of the non-classical phenomena in complex states involving a large number of particles also has another fundamental motivation. There is still a debate about the transition between the quantum and the classical realms. While it is commonly agreed that decoherence is a necessary step in the measurement process, one might still think that additional processes not predicted by quantum mechanics are present on a big enough scale that give rise to objective outcomes of the measurement. Therefore, one could potentially see the indirect signatures of such phenomena in these intermediate scales, if one predicts non-classical effect but experimentally observes its disappearance with the system size.

This dissertation explores problems of non-classicality in the limits of macroscopic numbers of photons and the mesoscopic description of non-classical phenomena of bosonic fields. In particular, the work concentrates on entanglement, Bell non-classicality and contextuality. The work is structured as follows: Section II presents preliminary information on the problems investigated, Section III provides an overview of the results presented in the articles, and Section V presents perspectives for further research.

II. PRELIMINARIES

Let us first recall some concepts that will provide context and notation conventions for the summarized results of the series of papers presented as part of the PhD dissertation.

A. Entanglement in quantum field theory

To discuss the entanglement, it is necessary to introduce the state space of the theory. Let us briefly review how the state space is constructed in both first and second quantizations.

1. *First quantization state space and entanglement*

In first quantization, for problems involving point quantum particles in space, one can describe the pure state of a single particle by a normalized vector $|\psi\rangle$ in the single-particle Hilbert space $\mathcal{H}$. This vector can be associated with the wave function $\psi(\vec{r})$ in the position representation, which is interpreted as providing probability density of finding a particle at a given position through the Born rule $dP(\vec{r}) = |\psi(\vec{r})|^2 d\vec{r}$. Therefore, one chooses the Hilbert space $\mathcal{H}$ to be isomorphic to the space of square-integrable functions $L^2(\mathcal{M})$ or its subspace singled out by the evolution equation. Here, $\mathcal{M}$ is some flat 3-dimensional manifold on which the particle is considered. One can show $L^2(\mathcal{M})$ to be separable. This property ensures that one can construct a countable basis in Hilbert space $\mathcal{H}$. Then, mixed states (density operators) $\hat{\rho}$ can be defined as bounded positive operators on space $\mathcal{H}$ with trace 1.

A state space of two distinct particles lives in a tensor product of single-particle spaces $\mathcal{H}_1 \otimes \mathcal{H}_2$. For pure states, one can characterize bipartite entanglement in terms of Schmidt decomposition. Any state $|\psi_{12}\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ can be decomposed as follows [36]:

$$|\psi_{12}\rangle = \sum_t \lambda_t \, |\phi_t\rangle_1 \otimes |\varphi_t\rangle_2 \,, \tag{1}$$

where coefficients $\lambda_t \geq 0$ fulfil relation $\sum_t |\lambda_t|^2 = 1$, and vectors $|\phi_t\rangle_1 \in \mathcal{H}_1$, $|\varphi_t\rangle_2 \in \mathcal{H}_2$ form two sets of orthonormal vectors, that is, $\langle \phi_t | \phi_{t'} \rangle_1 = \langle \varphi_t | \varphi_{t'} \rangle_2 = \delta_{t,t'}$. Here, $\delta_{t,t'}$ denotes the Kronecker delta. An important feature of Schmidt decomposition is that it is unique up to choice of the phase of the vectors $|\phi_t\rangle_1$, $|\varphi_t\rangle_2$. Still, phase relations between different terms $|\phi_t\rangle_1 \otimes |\varphi_t\rangle_2$ are unique. Now, the pure state is separable if there exists only one $\lambda_t \neq 0$, that is if it is a product state $|\phi_t\rangle_1 \otimes |\varphi_t\rangle_2$. If the state is not separable, it is entangled. For mixed state, one has that the state is separable if it can be put as a convex combination of product states of the subsystems:

$$\hat{\rho} = \sum_i p_i \hat{\rho}_i^1 \otimes \hat{\rho}_i^2, \tag{2}$$

where p_i can be interpreted as a probability of preparing product state $\hat{\rho}_i^1 \otimes \hat{\rho}_i^2$, and $\hat{\rho}_i^j$ denotes some density operator on j-th Hilbert space. Analogously, if $\hat{\rho}$ is not separable, it is entangled.

2. Second quantization state space and entanglement

In quantum field theory, one constructs the Fock space. One can build an orthonormal basis for this space starting from the vacuum state $|\Omega\rangle$, which is assumed to contain no particles in any mode. Next, one introduces creation (annihilation) operators $\hat{a}_i^\dagger$ ($\hat{a}_i$) which add (remove) a single particle in some single-particle state $|a_i\rangle$ (which defines a mode, in the field theoretic language). If states $|a_i\rangle$ form an orthonormal basis in the Hilbert space $\mathcal{H}$ of single particle states, then creation and annihilation operators fulfill canonical commutation relations for bosons or anticommutation relations for fermions:

$$[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{i,j}, \;\; [\hat{a}_i, \hat{a}_j] = [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0, \tag{3}$$

$$\{\hat{a}_i, \hat{a}_j^\dagger\} = \delta_{i,j}, \;\; \{\hat{a}_i, \hat{a}_j\} = \{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} = 0. \tag{4}$$

All elements of the Fock basis are obtained by applying all possible monomials of these creation operators with a proper normalization factor to $|\Omega\rangle$:

$$|n_1, n_2, ...\rangle = \frac{(\hat{a}_1^\dagger)^{n_1} (\hat{a}_2^\dagger)^{n_2} ...}{\sqrt{n_1! n_2! ...}} \, |\Omega\rangle \,, \tag{5}$$

where n_i denotes the number of particles in i-th mode. For bosons and fermions one has $\sum_i n_i < \infty$ while *additionally* for fermions $n_i \in \{0, 1\}$. Importantly, this basis is countable [37] because one has a countable number of modes, and the modes always contain a finite number of particles. Let us remark that the choice of the creation and annihilation operators is not unique. If we decide to use another basis for single-particle states, say $|d_k\rangle = \sum_i u_{ki} \, |a_i\rangle$ then one can introduce creation operators associated with this basis $\hat{d}_k^\dagger = \sum_i u_{ki} \hat{a}_i^\dagger$. These operators, together with their conjugates, form an identical (anti)commutator algebra as $\hat{a}_i$, $\hat{a}_i^\dagger$.

Various types of entanglement can be analyzed in the Fock space [38–40]. Here we consider the type of entanglement of quantum fields that can be directly observed. This entanglement is called the mode entanglement. To study entanglement, one has to specify at least two distinguishable subsystems. While in the Fock space specific particles cannot be distinguished by the construction, one can distinguish different orthogonal modes. Thus, consider the division of modes into two families of mutually orthogonal modes, first given by the set of modes $\{a_i\}$, and the second by $\{b_l\}$. Now, let each family of modes constitute a subsystem. Then, some pure state $|\psi_{ab}\rangle$ from the considered Fock space is separable if it can be written as:

$$|\psi_{ab}\rangle = F(\{a_i^\dagger\})G(\{b_l^\dagger\})\,|\Omega\rangle\,, \tag{6}$$

where $F(\{a_i^\dagger\})$ stands for some polynomial of creation operators in modes $\{a_i\}$ and analogously $G(\{b_l^\dagger\})$ for modes $\{b_l\}$. For the mixed state, one has that the state of field $\hat{\rho}_F$ is separable if it can be put as a convex combination of separable pure states:

$$\hat{\rho}_F = \sum_j p_j\,|\psi_j\rangle\,\langle\psi_j|\,, \tag{7}$$

where all states $|\psi_j\rangle$ have a form (6). Once again, the state is entangled if it is not separable.

3. *Entanglement criteria for quantum optical fields*

Let us concentrate on optical fields. The important question is how one can access information about whether the state of the field is $\hat{\rho}_F$ entangled. In the case of polarization entanglement, one of the tools for this task are the Stokes operators [33, 41]. These operators are quantum-optical analogues of the Stokes parameters commonly used in classical electrodynamics for the description of polarization. One obtains Stokes operators from Stokes parameters by choosing a quantum model for the intensity of light. If we consider a specific beam (spatial mode) and model intensity by number of photons, the Stokes operators read:

$$\hat{\Theta}_i = \hat{a}_i^\dagger\hat{a}_i - \hat{a}_{i\perp}^\dagger\hat{a}_{i_\perp}. \tag{8}$$

Here, $\hat{a}_i$ and $\hat{a}_{i\perp}$ are annihilation operators in two orthogonal polarization modes, and $i = 1, 2, 3$ stands for three mutually unbiased bases for the considered optical modes. In the description of polarization, these basis modes could be chosen as:

- $i = 1$ right-handed and left-handed circular polarisation, $\{R, L\}$,
- $i = 2$ diagonal and anti-diagonal polarisation, $\{D, A\}$,
- $i = 3$ horizontal and vertical polarisation $\{H, V\}$.

In addition, one considers the operator $\Theta_0 = \hat{a}_i^\dagger\hat{a}_i + \hat{a}_{i\perp}^\dagger\hat{a}_{i_\perp}$ that describes the total number of photons in the beam defined by a single spatial (propagation) mode.

An interesting feature of these operators is that whenever one restricts oneself to states from the subspace where only a single photon is present in the modes, Stokes operators act on these states exactly as Pauli matrices $\hat{\sigma}_i$ on a qubit. This gives a motivation that Stokes operators could be used to construct criteria for entanglement concerning discrete degrees of freedom. In fact, a broad class of such criteria can be obtained. This is because it was shown that from any entanglement indicator for multi-qubit systems, which can be constructed using tensor products of Pauli matrices, one can obtain an entanglement indicator for the field by mapping $\hat{\sigma}_i^X \to \hat{\Theta}_i^X$ [42]. Here, the superscript X denotes the subsystem on which the given operator acts.

An alternative to Stokes operators are normalized Stokes operators [34, 43], which in the situation as considered above read:

$$\hat{S}_i = \hat{\Pi}\frac{\hat{n}_i - \hat{n}_{i_\perp}}{\hat{n}_i + \hat{n}_{i_\perp}}\hat{\Pi}, \tag{9}$$

where $\hat{\Pi} = \mathbb{1} - |0,0\rangle\langle 0,0|$ is a projector into states which has at least a single photon, and $\hat{n}_{i(i\perp)}$ are photon number operators. The operator $\hat{\Pi}$ additionally plays the role of the operator $\hat{S}_0$ replacing $\hat{\Theta}_0$. These operators have a bounded spectrum given by rational numbers from the interval $[-1,1]$. This fact is useful in considerations of Bell inequalities, which we discuss later. Importantly, for normalized Stokes operators, one has an analogous mapping of entanglement indicators using $\hat{\sigma}_i^X \to \hat{S}_i^X$. It is important to note that while Stokes parameters are associated with polarization, one can use Stokes operators for the description of any two orthogonal modes, which do not have to be polarization modes.

B. Entanglement in squeezed states

For decades one of the primary sources of entangled photons has been the parametric down-conversion process (PDC) [44, 45]. It is a process that can occur in non-linear medium (e.g., BBO crystal). In PDC photon from the pumping field with wave vector $\vec{k}_p$ and frequency ω_p can be annihilated, which is followed by the creation of a pair of photons with wave vectors $\vec{k}_s, \vec{k}_i$ and frequencies ω_s, ω_i. These pairs of photons have to follow a phase matching conditions, which tend to approximate momentum and energy conservation between the pump photon and the created pair:

$$\vec{k}_p \approx \vec{k}_s + \vec{k}_i, \tag{10}$$

$$\omega_p \approx \omega_s + \omega_i. \tag{11}$$

These conditions are a consequence of the superposition of the emission of the pairs of photons in the entire volume of the crystal illuminated by the pump field. In the specific case of type I phase matching with created photons having the same energy and polarization, these photons are propagating on a cone. This is a result of momentum conservation (phase matching condition concerning momentum), which requires that components of the momentum of created photons that are perpendicular to the momentum of pump photon are opposite. In the parametric approximation, in which one treats the pumping field classically, this process of creation of particle pairs into two phase-matched modes a and b can be to a good approximation described by the interaction Hamiltonian:

$$\hat{H} = \gamma \hat{a}^\dagger \hat{b}^\dagger + h.c., \tag{12}$$

where parameter γ is related to the intensity of the pumping field. The state obtained by the unitary evolution of the vacuum imposed by $\hat{H}$ is called a two-mode squeezed vacuum state [46]. One can show that this state is entangled. However, one can also obtain different types of entangled states from this process. In particular, for a weak pumping, it can be used to obtain approximately singlet states encoded in polarization or paths. Assume for now that photons in created pairs have orthogonal polarization to each other (PDC type II phase matching) and have the same energy. Then, due to the birefringence of the non-linear crystal (only birefringent crystals have high enough quadratic non-linearity to get a PDC effect), the photons are no longer propagating on the surface of a single cone. The different refractive index for the differently polarized photons results in wave vectors $\vec{k}_s, \vec{k}_i$ of not equal length. For a specific orientation of the crystal, the created photon pairs propagate on two cones. There are two lines on which the cones intersect. Then one can extract two beams of light from the intersections of the cones. In such a scenario, one cannot specify the polarization of the beams, as a photon of a given polarization was created in each beam with the same probability. Let us choose these two polarizations to be H and V, and denote the modes of the first beam as a_H, a_V and of the second beam as b_H, b_V. Then, the effective interaction Hamiltonian for this process can be put in the following form

$$\hat{H}_{2\times 2} = \gamma \hat{a}_V^\dagger \hat{b}_H^\dagger - \gamma \hat{a}_H^\dagger \hat{b}_V^\dagger + h.c.. \tag{13}$$

Note that this Hamiltonian is simply a sum of two two-mode squeezing Hamiltonians (12). Applying unitary $\exp\left(-i\hat{H}_{2\times 2} t/\hbar\right)$ to vacuum one obtains the 2×2 mode squeezed vacuum state. It can be explicitly written as:

$$|\psi_-\rangle = \frac{1}{\cosh^2(\Gamma)} \sum_{n=0}^{\infty} \tanh^n(\Gamma) \sum_{m=0}^{n} (-1)^m |(n-m), m; m, (n-m)\rangle$$
$$= \frac{1}{\cosh^2(\Gamma)} \sum_{n=0}^{\infty} \sqrt{n+1} \tanh^n(\Gamma) \left|\psi_-^n\right\rangle . \quad (14)$$

where $\Gamma = \gamma t/\hbar$ is called amplification gain. A bright, i.e., with high Γ, state we shall call a bright squeezed vacuum state (BSV). Here we used the notation for Fock states with occupation numbers given for the following order of modes: a_H, a_V, b_H, b_V. Observe that $\left|\psi_-^1\right\rangle$ is simply a two-photon polarization singlet state. Therefore, for a weakly pumped crystal, i.e., for small Γ the BSV state is effectively a superposition of the singlet state and the vacuum. In fact, it inherits many features of the singlet state, such as for example, EPR-like anti-correlations and rotational invariance with respect to simultaneous action of the same local transformation of basis modes in both parties. In other words, the form of the state is the same in any common choice of polarization basis for both parties. In addition, this state with an undefined number of photons can be generated to possess large average numbers of photons [47]. Because of all of that, it is sometimes referred to as the "macroscopic singlet".

One can also obtain entangled states that have an undefined number of photons using generalization of two-mode squeezing to a higher number of modes. Consider three modes a_1, b_1 and c_1 and the following interaction Hamiltonian in a parametric approximation:

$$\hat{H} = \gamma \hat{a}_1^\dagger \hat{b}_1^\dagger \hat{c}_1^\dagger + h.c.. \quad (15)$$

This Hamiltonian seems to generalize Hamiltonian (12). Experimental realizations of such interactions have recently been presented [48]. However, this description in terms of the parametric approximation is pathological, as $\exp\{-i\hat{H}t/\hbar\}$ is not a proper unitary operator in Fock space. Let us remark that one could restore unitarity by considering the pump field also as quantized [49].

Similarly to the construction of the BSV state, one could (keeping in mind the problems with (15)) consider the state of six orthogonal modes generated from the vacuum by the sum of two such Hamiltonians:

$$\hat{H}_{GHZ} = \gamma \hat{a}_1^\dagger \hat{b}_1^\dagger \hat{c}_1^\dagger + \gamma \hat{a}_2^\dagger \hat{b}_2^\dagger \hat{c}_2^\dagger + h.c.. \quad (16)$$

This process was first considered in the work co-authored by the author of this thesis [50]. Here, one can think as an example that sets of modes $\{a_1, a_2\}$, $\{b_1, b_2\}$ and $\{c_1, c_2\}$ describe now three beams, where each is propagated to one of the three separate parties. This state is, in fact, a genuinely tripartite entangled state [50]. What is more, it generalizes a GHZ state to a state with an undefined number of photons in the analogous manner to how the BSV state generalizes a singlet state. Therefore, it is called the bright GHZ state (BGHZ). This state can be written in the Fock basis as:

$$\begin{aligned} |BGHZ\rangle &= \sum_{k=0}^{\infty} \sum_{m=0}^{k} C_{k-m}(\Gamma) C_m(\Gamma) (\hat{a}_1^\dagger \hat{b}_1^\dagger \hat{c}_1^\dagger)^{k-m} (\hat{a}_2^\dagger \hat{b}_2^\dagger \hat{c}_2^\dagger)^m |\Omega\rangle \\ &= \sum_{k=0}^{\infty} \sum_{m=0}^{k} C_{k-m}(\Gamma) C_m(\Gamma) |k-m, m; k-m, m; k-m, m\rangle , \end{aligned} \quad (17)$$

where $C_q(\Gamma)$ are complex coefficients dependent on Γ. Let us comment that finding a general form of these coefficients still poses an open problem. This is because a parametric approximation is not well suited for a proper description of the generation of this state, as the series expansion of $\exp\left(-i\hat{H}_{GHZ}t/\hbar\right)$ does not lead to a normalizable state (i.e., $\exp\left(-i\hat{H}_{GHZ}t/\hbar\right)$ is not unitary). This problem is analogous to the problem of the generalization of single-mode squeezing with Hamiltonians $\gamma(a^\dagger)^n + h.c.$ for $n > 2$

[49]. However, one can approximately calculate $C_q(\Gamma)$ for $\Gamma < 0.9$ using the series expansion to calculate the Padé approximants [50] which we briefly discuss below.

Consider first the Hamiltonian $\hat{H}_1 = \gamma \hat{a}_1^\dagger \hat{b}_1^\dagger \hat{c}_1^\dagger + h.c.$. In the standard approach, this Hamiltonian would produce the following state from the vacuum:

$$|\Sigma_1\rangle = e^{-iH_1 t/\hbar} |\Omega\rangle = \sum_{k=0}^{\infty} c_k (\hat{a}_1^\dagger \hat{b}_1^\dagger \hat{c}_1^\dagger)^k |\Omega\rangle \,, \tag{18}$$

where second equality is obtained through series expansion of the exponent. Here, coefficients c_k are given by:

$$c_k = \sum_{l=0}^{\infty} \frac{(-i\Gamma)^{k+2l}}{(k+2l)!} P_{k+2l}^k, \tag{19}$$

where P_l^k fulfil the recurrence relation: $P_l^k = P_{l-1}^{k-1} + (k+1)^3 P_{l-1}^{k+1}$ with conditions $P_l^k = 0$ if $k > l$ and $P_k^k = 1$. One can find that the norm of c_k is divergent, and so this approach itself does not allow one to obtain probability amplitudes for the state. However, one can calculate Padé approximants for this series expansion, which allows avoiding the divergent approximation. This approximation is built to approximate the function (probability amplitude) with the rational function rather than the power series. In this approach, one obtains that the evolution of vacuum approximately results in the state:

$$|\Sigma_1\rangle = \sum_{k=0}^{\infty} C_k(\Gamma) (\hat{a}_1^\dagger \hat{b}_1^\dagger \hat{c}_1^\dagger)^k |\Omega\rangle \,, \tag{20}$$

where $C_k(\Gamma)$ are rational functions:

$$C_k(\Gamma) = \frac{\sum_{n=0}^{N} X_n^k (-i\Gamma)^n}{\sum_{m=0}^{M} Y_m^k (-i\Gamma)^m}, \tag{21}$$

where $[N/M]$ describes the degree of approximation. The coefficients X_n^k, Y_m^k are chosen so that the first $(N+M+1)$ terms of the Taylor series expansion of $C_k(\Gamma)$ are the same as first $(N+M+1)$ terms of (19). Then, these $C_k(\Gamma)$ are used to approximate the BGHZ state 17. This is because $\hat{H}_{GHZ} = \hat{H}_1 + \hat{H}_2$, where $\hat{H}_2$ is analogous to $\hat{H}_1$ for modes with subscript 2. The BGHZ state is simply a product state built from $|\Sigma_1\rangle$ and $|\Sigma_2\rangle$. Note that while it is a separable state in bipartition into modes a_1, b_1, c_1 and a_2, b_2, c_2, this does not prevent the state from being entangled in different partitions. Further down we shall be interested in partition a_1, a_2 and b_1, b_2 and finally c_1, c_2 (effectively modes leading to three separate observation stations) in which state is not factorizable.

C. Bell non-classicality

One of the most remarkable effects which originate from entanglement is the Bell non-classicality. The work of Bell [51] showed that quantum mechanics is fundamentally incompatible with the local realistic description advocated by Einstein [1] and followers. This was achieved by showing that predictions of quantum mechanics violate an inequality which has to be fulfilled by the local hidden variable models. Such types of inequalities, in general, are called Bell inequalities. Let us discuss this incompatibility based on the widely known CHSH inequality [52].

1. CHSH inequality

Consider two spatially separated parties A and B which can perform measurements, each choosing between two different measurement settings. The parties chose their settings randomly and independently of each other. Let us denote the settings for party A as A_1, A_2 and for party B analogously as B_1, B_2. Furthermore, let us assume that each measurement has two possible outcomes ± 1. Then, parts of some system are distributed to the parties upon which they perform measurement. Suppose that the measurement process in both parties finishes before any information about the chosen setting traveling with the speed of light could reach another party. The key assumption for deterministic LHV models is that all the results of the measurements are determined by some local hidden variables which we denote as λ. Here, locality manifests itself in the sense that any local operations (choice of measurement setting) performed on subsystem A (B) do not impact results in subsystem B (A). This is motivated by the fact that in this scenario information about local operations cannot reach the other party within laws of relativity, and thus classically results should be determined only by the local variables. We note that results of the parties in LHV models can depend on each other by classical correlations imposed by a (hidden) common cause λ during the preparation of the system. Let us denote the result of the measurement in party X for a given setting X_i conditioned on the configuration of hidden variables as $R_X(i, \lambda)$. One can check that for given λ:

$$\Big[R_A(1,\lambda) + R_A(2,\lambda)\Big] R_B(1,\lambda) + \Big[R_A(1,\lambda) - R_A(2,\lambda)\Big] R_B(2,\lambda) = \pm 2. \tag{22}$$

This expression is a random variable, and thus one can calculate its expectation value over some probability distribution $\rho(\lambda)$ which determines the distribution of local hidden variables supposedly related to the state of the full system. Note that, one is not able to measure in one run results for all settings. Thus, in the experiment, one cannot directly have access to this random variable. However, one can separately obtain expectation values for different terms of (22) since all involve only a single configuration of settings. Finlay, due to the linearity of the operation of averaging over probability distribution, the result has to coincide with the expectation value for this inaccessible random variable. Now, clearly, using the fact that $\int \rho(\lambda) d\lambda = 1$, and due to the equality (22) we have that

$$|\langle CHSH \rangle| \equiv \Big| \langle R_A(1,\lambda) R_B(1,\lambda) \rangle_{LHV} + \langle R_A(2,\lambda) R_B(1,\lambda) \rangle_{LHV} + \langle R_A(1,\lambda) R_B(2,\lambda) \rangle_{LHV} - \langle R_A(2,\lambda) R_B(2,\lambda) \rangle_{LHV} \Big| \leq 2. \tag{23}$$

Here, $\langle R_A(i,\lambda) R_B(j,\lambda) \rangle_{LHV}$ stands for the expectation value for some local hidden variable distribution $\rho(\lambda)$. These expectation values are called correlation functions. As we did not make any assumptions on the distribution $\rho(\lambda)$ this inequality should hold for any state according to deterministic LHV models. This inequality is called the CHSH inequality. In fact, one can also show that this inequality also holds for stochastic LHV models. In such models, one assumes more generally that the outcomes can be randomly distributed for given λ, i.e., one has a probability distribution of local results $P(R_X | i, \lambda)$ conditioned on the choice of setting and λ instead of definite values of $R_X(i, \lambda)$. The locality in such models is realized by the assumption of factorization of joint probabilities:

$$P(R_A, R_B | i, j, \lambda) = P(R_A | i, \lambda) P(R_B | j, \lambda). \tag{24}$$

Let us now analyze the example of predictions of quantum mechanics for this kind of scenario. Consider that the source prepares a singlet state encoded in polarization $\left|\psi_-^1\right\rangle$ (see (14)) and distributes one beam to each party. Parties have polarization analyzers that they can rotate by some angle α to measure in different linear polarization basis. Assigning rotation angle 0 to the $\{H, V\}$ polarization basis one can describe creation operators in rotated measurement basis of party A as:

$$\begin{aligned} \hat{a}^\dagger(\alpha) &= \cos\alpha\ \hat{a}_H^\dagger + \sin\alpha\ \hat{a}_V^\dagger \\ \hat{a}_\perp^\dagger(\alpha) &= -\sin\alpha\ \hat{a}_H^\dagger + \cos\alpha\ \hat{a}_V^\dagger, \end{aligned} \tag{25}$$

and analogously for party B with $\hat{a}^\dagger_{H(V)} \rightarrow \hat{b}^\dagger_{H(V)}$. Then, suppose that the parties assign the result 1 to events where a single photon is detected in the first basis mode and -1 in the opposite case. Let party A choose between two settings given by the angles $\alpha_{A1} = 0$, $\alpha_{A2} = \pi/4$, and party B between $\alpha_{B1} = \pi/8$ and $\alpha_{B2} = -\pi/8$. This scenario matches exactly the CHSH scenario. One can directly calculate appropriate quantum expectation values for this setup to evaluate the left hand side of inequality (23). In the result, one obtains $2\sqrt{2} \leq 2$, and therefore the inequality is violated showing incompatibility of the predictions of quantum mechanics with LHV models.

2. *CHSH-like inequality for optical fields*

One can also build a CHSH-like inequality for general four-mode quantum optical fields using normalized Stokes operators (9). In such a case, one considers the possible results $R_X(i,\lambda)$ to be rational numbers contained in the interval $[-1,1]$. However, due to the fact that CHSH expression $\langle CHSH \rangle$ is linear in all $R_X(i,\lambda)$ it attains its extreme at the boundary, i. e., when $R_X(i,\lambda) = \pm 1$. Therefore, for such a case one has an unchanged inequality fulfilled by the LHV models. Then, one can see that the normalized Stokes operators provide such a measurement with results being rational numbers on the considered interval. Then, in quantum analysis, instead of expectation values $\langle R_A(i,\lambda) R_B(j,\lambda)\rangle_{LHV}$ one can consider the quantum expectation values $\langle \hat{S}^A(i)\hat{S}^B(j)\rangle$ where $\hat{S}^X(i)$ stands for a normalized Stokes operator constructed in the basis corresponding to the i-th setting. In the measurement basis from the above example, they are given for party A by:

$$\hat{S}^A(i) = \hat{\Pi}\frac{\hat{a}^\dagger(\alpha_{A_i})\hat{a}(\alpha_{A_i}) - \hat{a}_\perp^\dagger(\alpha_{A_i})\hat{a}_\perp(\alpha_{A_i})}{\hat{a}^\dagger(\alpha_{A_i})\hat{a}(\alpha_{A_i}) + \hat{a}_\perp^\dagger(\alpha_{A_i})\hat{a}_\perp(\alpha_{A_i})}\hat{\Pi}. \tag{26}$$

Then choosing the same rotation angles as for the case of the singlet state, one can show a violation of the considered CHSH-like inequality using the BSV state (14).

Let us comment that early attempts to construct Bell inequalities for optical fields relayed on standard Stokes operators (8), which turned out to be an incorrect approach. In these attempts, one considers as a quantum correlation functions $\langle \hat{\Theta}^A(i)\hat{\Theta}^B(j)\rangle / \langle \hat{\Theta}_0^A \hat{\Theta}_0^B \rangle$ and tries to obtain violation of the, e.g., CHSH inequality based on them [53, 54]. However, inequalities obtained for this approach have in the derivation an additional assumption of *non-enhancement of intensity*. More precisely, the derivation assumes that the hidden variable that describes the total intensity of light is shared across all the choices of the local settings. In the result, the violation of such inequalities does not have to imply the violation of local realism. This is because the violation of this non-enhancement assumption could be the reason for observing the violation of inequality [55].

3. *CH inequality*

Let us additionally recall another fundamental Bell inequality, called the CH inequality [56]. This inequality is built directly from probabilities instead of correlation functions. Let us denote by $\mathcal{E}_i^X$ some event in the X-th party for the i-th setting. Then only from the properties of probability distributions and the locality assumption in terms of factorization of joint probabilities (24) one can find the CH inequality:

$$-1 \leq P(\mathcal{E}_1^A, \mathcal{E}_1^B) + P(\mathcal{E}_2^A, \mathcal{E}_1^B) + P(\mathcal{E}_2^A, \mathcal{E}_2^B) - P(\mathcal{E}_1^A, \mathcal{E}_2^B) - P(\mathcal{E}_2^A) - P(\mathcal{E}_1^B) \leq 0. \tag{27}$$

In fact, for the case where one has two possible outcomes per party, this inequality is equivalent to CHSH inequality [57]. To see this, let us choose all events $\mathcal{E}_i^X$ to be that for a given setting one oberves result -1. Then, the correlation function:

$$\langle R_A(i,\lambda)R_B(j,\lambda)\rangle_{\rho(\lambda)} = P(R_A = R_B|i,j) - P(R_A \neq R_B|i,j), \tag{28}$$

can be rewritten as:

$$\langle R_A(i,\lambda)R_B(j,\lambda)\rangle_{\rho(\lambda)} = 4P(\mathcal{E}_i^A, \mathcal{E}_j^B) - 2P(\mathcal{E}_i^A) - 2P(\mathcal{E}_j^B) + 1. \tag{29}$$

Inserting this to the CHSH expression in (23) one can retrieve the CH inequality (27). Thus, a violation of one inequality is accompanied by the violation of the second one. One also has a general relation, valid also for quantum predictions, between the values of the $\langle CHSH\rangle$ and the CH expression, which we denote as $\langle CH\rangle$:

$$\langle CH\rangle = \frac{\langle CHSH\rangle}{4} - \frac{1}{2}. \tag{30}$$

However, in general, CH inequality is not equivalent to CHSH-like inequalities derived for a higher number of possible outcomes. If one derives quantum optical Bell inequality based on intensity rates CH and CHSH-like forms of these are not equivalent. One has to modify the CHSH inequality to become equivalent to the CH one (e.g., [58] for the case of inefficient detection)

D. Contextuality

Quantum mechanics is also not compatible with classical concept represented by non-contextual hidden variable models. Let us briefly discuss the underlying classical intuition behind such a class of hidden variable models. In quantum mechanics non-degenerate observables define the context of degenerate ones (which are functions of the former ones), but not in a unique way. A degenerate observable may commute (be jointly measurable) with infinitely many non-degenerate ones. Thus, it can be measured within many contexts. Is it possible to model quantum mechanics with hidden predetermined values of measurement in such a way that functional relations between all jointly measurable observables are satisfied, and the predetermined values of degenerate observable do not depend on context?

The incompatibility of this class of hidden variable models with quantum mechanics was first shown also by Bell [59] and independently by Kochen and Specker [60]. This result is commonly known as Kochen-Specker theorem. Let us present this incompatibility using the simple method presented by Peres [61] and Mermin [62, 63]. Quantum mechanics represents the values $V(O_i)$ as eigenvalues of Hermitian operators representing observables $\hat{O}_i$ which are the only possible outcomes of measurement of these observables. Importantly, the sets of compatible observables in quantum description translate into the sets of mutually commuting observables. Now, if a set of compatible observables, e.g., let us assume this set to be $\hat{O}_i$ for $i \leq n$, fulfills some relation:

$$f(\hat{O}_1, ...\hat{O}_n) = 0, \tag{31}$$

the same relation must be fulfilled by each configuration of eigenvalues $V(O_i)$. Consider now the following table of observables $\hat{A}_{ij}$ for two-qubit systems called the Peres-Mermin square:

$\hat{A}_{ij}$	$j=1$	$j=2$	$j=3$
$i=1$	$\hat{\sigma}_3^1\hat{\sigma}_0^2$	$\hat{\sigma}_0^1\hat{\sigma}_3^2$	$\hat{\sigma}_3^1\hat{\sigma}_3^2$
$i=2$	$\hat{\sigma}_0^1\hat{\sigma}_1^2$	$\hat{\sigma}_1^1\hat{\sigma}_0^2$	$\hat{\sigma}_1^1\hat{\sigma}_1^2$
$i=3$	$\hat{\sigma}_3^1\hat{\sigma}_1^2$	$\hat{\sigma}_1^1\hat{\sigma}_3^2$	$\hat{\sigma}_2^1\hat{\sigma}_2^2$

One can check that operators $\hat{A}_{ij}$ with repeating indices commutes. Therefore, all rows and all columns provide sets of compatible observables. In fact, the product of operators in each row results in identity, and the same holds for the first two columns. However, the product of operators in the last column is equal to minus identity. Consider a product of hypothetical $V(A_{ij})$ for each row:

$$\Big[V(A_{11})V(A_{12})V(A_{13})\Big]\Big[V(A_{21})V(A_{22})V(A_{23})\Big]\Big[V(A_{31})V(A_{32})V(A_{33})\Big] = 1, \tag{32}$$

where the equality is obtained as based on the discussed relations each square bracket has to be equal to 1. Now, repeating the same for columns, one gets:

$$\Big[V(A_{11})V(A_{21})V(A_{31})\Big]\Big[V(A_{12})V(A_{22})V(A_{32})\Big]\Big[V(A_{13})V(A_{23})V(A_{33})\Big] = -1, \tag{33}$$

where minus appears due to the expression in the last square bracket. Multiplying these equations by sides, one has on the left-hand side the product of positive expressions $V(A_{ij})^2$ while on the right-hand side, one has -1. Thus, one gets a contradiction, showing the incompatibility of non-contextual hidden variable models with quantum mechanics.

Notice that the prediction based on the Peres-Mermin square is completely state-independent. This is in contrast to the case of the Bell Theorem where one relied on the specific quantum property of some states to show the incompatibility with local realistic hidden variable models. Here, however, the argument is solely based on the properties of the observables.

The predictions of quantum mechanics also in the case of contextuality turned out to be better suited for the description of nature. This is because experimental efforts allowed for falsifying non-contextual description [64, 65]. Besides the fundamental relevance, the problem of contextuality has also recently gained interest, as it could be the key feature that enables advantage in quantum computation [66, 67] and communication tasks [68].

E. Open dynamics and reduced state of the field description

In general, the full quantum description of complex systems becomes quickly infeasible with increasing system size. This is in particular true when one deals with infinite-dimensional systems involving states with an undefined number of particles. The complexity of the analysis also increases; as in any practical scenario, one has to consider the decoherence effects imposed on the system by the interaction with the environment. Therefore, one of the important problems is to find mesoscopic descriptions of such systems, which simplify the analysis but still allow obtaining proper predictions about relevant degrees of freedom in situations where quantum effects play an essential role.

One of the recently proposed mesoscopic descriptions of bosonic systems is the reduced state of the field (RSF) approach [69]. The RSF formalism seeks simplification of the description by reducing the infinitely dimensional framework of the second quantization to a finite-dimensional, single-particle-like Hilbert space typical of the first quantization. Let us recall the construction of RSF.

Consider some density operator $\hat{\rho}_F$ on the Fock space of N orthogonal modes $\{a_k\}_{k=1}^N$. The RSF reduces this state to two structures on the N-dimesional Hilbert space with orthonormal basis $\{|k\rangle\}_{k=1}^N$ related to the described modes ($|k\rangle$ is designated to describe mode a_k). These structures are: single-particle density matrix and averaged field:

$$\hat{\rho} = \sum_{k,k'=1}^{N} \mathrm{tr}\Big\{\hat{\rho}_F \hat{a}_{k'}^\dagger \hat{a}_k\Big\} |k\rangle\langle k'|, \quad |\alpha\rangle = \sum_{k=1}^{N} \mathrm{tr}\{\hat{\rho}_F \hat{a}_k\} |k\rangle . \tag{34}$$

Observe that $\hat{\rho}$ after normalization has all the mathematical properties of the density matrix. Similarly $|\alpha\rangle$ after normalization could be seen as a pure state. However, these reduced states are not real states and do not have the typical probabilistic interpretation. Instead, the operator $\hat{\rho}$ depicts the occupation of modes and coherences, and $|\alpha\rangle$ gives access to information about the local phases of the field. One also associates observables on single-particle-like Hilbert space with a specific class of observables on the Fock space:

$$\hat{O} = \sum_{k,k'=1}^{N} o_{k,k'} a_k^\dagger \hat{a}_{k'} \leftrightarrow \hat{o} = \sum_{k,k'=1}^{N} o_{k,k'} \left|k\right\rangle \left\langle k'\right|. \tag{35}$$

Importantly, this association (reduction) of observables preserves the expectation values:

$$\mathrm{tr}\left\{\hat{\rho}_F \hat{O}\right\} = \mathrm{tr}\{\hat{\rho}\hat{o}\}. \tag{36}$$

The important feature of RSF is that it allows for the consideration of the open evolution of the reduced states. Often, the open evolution that the system undergoes can be described as roughly Markovian. In such circumstances, the evolution of the state $\hat{\rho}_F$ is given by the GKLS equation [70, 71]. One can consider a class of such equations that describe particle decay and production, random elastic scattering, and classical coherent pumping. These equations, using the independent particles approximation, can be generally put as [69, 72]:

$$\begin{aligned}\frac{d}{dt}\hat{\rho}_F &= -\frac{i}{\hbar}[\hat{H}, \rho_F] + \sum_k^N [(\xi_k \hat{a}_k^\dagger - \xi_k^* \hat{a}_k), \hat{\rho}_F] + \sum_j \kappa_j (\hat{U}_j \hat{\rho}_F \hat{U}_j^\dagger - \hat{\rho}_F) \\ &+ \sum_{k,k'=1}^{N} \Gamma_\downarrow^{k',k} \left(\hat{a}_k \hat{\rho}_F \hat{a}_{k'}^\dagger - \frac{1}{2}\{\hat{a}_{k'}^\dagger \hat{a}_k, \hat{\rho}_F\}\right) + \sum_{k,k'=1}^{N} \Gamma_\uparrow^{k',k} \left(\hat{a}_{k'}^\dagger \hat{\rho}_F \hat{a}_k - \frac{1}{2}\{\hat{a}_k \hat{a}_{k'}^\dagger, \hat{\rho}_F\}\right),\end{aligned} \tag{37}$$

where Hamiltonian $\hat{H} = \sum_{k,k'} \omega_{k,k'} \hat{a}_k^\dagger \hat{a}_{k'}$, complex parameters ξ_k describe classical pumping field, κ_j describes probability distribution of scattering processes described by unitary transformations of annihilation operators $\hat{U}_j^\dagger \hat{a}_k \hat{U}_j = \sum_{k'} u_{k',k}^j \hat{a}_{k'}$ with u^j being unitary matrix, and $\Gamma_\updownarrow^{k',k}$ are creation and annihilation rates. For this class of evolution equations, one can find the corresponding evolution equations for $\hat{\rho}$, $\left|\alpha\right\rangle$:

$$\frac{d}{dt}\hat{\rho} = -\frac{i}{\hbar}[\hat{h}, \hat{\rho}] + (\left|\xi\right\rangle\left\langle\alpha\right| + \left|\alpha\right\rangle\left\langle\xi\right|) + \sum_j \kappa_j (\hat{u}_j \hat{\rho} \hat{u}_j^\dagger - \hat{\rho}) + \frac{1}{2}\{\hat{\gamma}_\uparrow - \hat{\gamma}_\downarrow^T, \hat{\rho}\} + \hat{\gamma}_\uparrow, \tag{38}$$

$$\frac{d}{dt}\left|\alpha\right\rangle = -\frac{i}{\hbar}\hat{h}\left|\alpha\right\rangle + \left|\xi\right\rangle + \sum_j \kappa_j (\hat{u}_j - 1)\left|\alpha\right\rangle + \frac{1}{2}(\hat{\gamma}_\uparrow - \hat{\gamma}_\downarrow^T)\left|\alpha\right\rangle, \tag{39}$$

where T stands for transposition, $\hat{h}$ is the reduced Hamiltonian obtained using (35) and:

$$\hat{\gamma}_\updownarrow = \sum_{k,k'} \Gamma_\updownarrow^{kk'} \left|k\right\rangle\left\langle k'\right|, \quad \left|\xi\right\rangle = \sum_k \xi_k \left|k\right\rangle, \quad \hat{u}_j = \sum_{k,k'} u_{k,k'}^j \left|k\right\rangle\left\langle k'\right|. \tag{40}$$

Additionally one can consider entropy within RSF:

$$S[\hat{\rho}; \left|\alpha\right\rangle] = k_B\, \mathrm{tr}\{(\hat{\rho}^\alpha + 1)\log(\hat{\rho}^\alpha + 1) - \hat{\rho}^\alpha \log(\hat{\rho}^\alpha)\}, \tag{41}$$

where $\hat{\rho}^\alpha = \hat{\rho} - \left|\alpha\right\rangle\left\langle\alpha\right|$ and k_B is the Boltzmann constant.

One can see the advantages of the RSF approach, as it inherits simple and intuitive first quantization structures and additionally as it is equipped with multiple tools for the analysis of the state. However, there are caveats to this description. For example, it was shown that while it is fully derived from quantum considerations, it is a highly classical description [72]. The described reductions are not appropriate for a description of entanglement. Furthermore, the entropy (41) possesses properties related to the semi-classical Wehrl entropy and not to the quantum von Neumann entropy. Observe that, as entanglement is one of the core resources for quantum information tasks, and the lack of it in the RSF makes this formalism not well-suited in this form for analysis of multiple relevant systems associated with such tasks.

III. OVERVIEW OF THE PRESENTED RESEARCH

A. General summary

Let us present a brief overview of the research included in this PhD thesis followed by a more in-depth summary of each article.

The first two articles [PhD1] and [PhD2] introduce two new sets of observables well suited for revealing non-clasicality of quantum optical fields for states with an undefined number of particles. In particular, they theoretically allow for observation of non-classical effects in the limits of high average numbers of photons. Both sets are inspired by Stokes operators. However, they try to achieve in a different way the goal of restoring some properties of Pauli matrices, most notably their bounded spectrum ± 1. In the first case of operators which we called the sign Stokes operators we try to mimic the action of the Pauli matrices on polarization optical qubits assigning result 1 (-1) to outcomes with a higher number of photons in the first (second) polarization mode. Finally, our procedure reduces the spectrum to three eigenvalues ± 1, 0 in contrast to all rational numbers for normalized Stokes operators. This gives the advantage in revealing Bell non-clasisicality for states with a higher average number of photons. In the second case, we try to build a new $\mathfrak{su}(2)$ representation which would also fulfill the anticommutation relations of Pauli matrices. This is in contrast to Stokes operators, which determine some $\mathfrak{su}(2)$ representation but do not fulfill this additional constraint. This set of operators allowed us, among other things, to propose generalization of the Peres-Mermin square for quantum optical fields that shows contextuality for macroscopically occupied states.

The third article [PhD3] shows that entanglement is fundamentally associated with Bell non-classicality not only for systems with a set number of particles but also for states with an undefined number of particles without constraints on the system size. To prove this claim, we introduce the Schmidt decomposition of the states in the Fock space. This decomposition itself provides a useful tool in the analysis of entanglement of quantum fields, and can give an insight into the methods required to reveal entanglement.

The last article [PhD4] provides a mesoscopic formalism for the description of bosonic systems and their open Markovian evolution. This formalism can be seen as the simplest extension of the reduced state of the field formalism that allows for entanglement considerations. In the core of this formalism lie particle number correlations which showed already their role in the entanglement of quantum optical fields through entanglement criteria based on Stokes operators. The proposed formalism reduces the problem of tracking state from infinite-dimensional Fock space to the evolution of a two-qudit density matrix upon which one can perform analysis using tools suited for finite-dimensional systems. Importantly, entanglement of the reduced two-qudit density matrix indicates entanglement of the full state of the bosonic field. Therefore, this formalism allows for easy and intuitive analysis of entanglement in bosonic systems. This includes highly occupied states with undefined photon particle number. This tool shows its versatility, as it can also describe other quantum effects such as, for example, sub-Poissonian statistics.

The joint effort of these works provides multiple tools for the analysis of various types of non-classicality of bosonic fields. What is more, using them one can reveal and analyze non-classicality both in scenarios in which only single particles are present and in scenarios considering highly occupied states.

B. New observables for detecting Bell non-classicality of quantum bosonic fields

While the problem of revealing Bell non-classicality of states of optical qubits is well studied, it is still underdeveloped for general states of a quantum optical field with undefined number of photons especially with a high average number of photons. The first approaches utilizing Stokes operators (8) were unsuccessful, and only recently utilization of normalized Stokes operators (9) led to proper Bell inequalities which do not treat in trivial way states with a higher number of photons. However, for states like BSV (14) and BGHZ (17) analysis with Bell inequality based on normalized Stokes operators reveals Bell non-classicality only in scenarios with a low average number of photons. One potential reason for that might be the fact that the eigenvalues of normalized Stokes operators for eigenstates $|n, m\rangle$ with the number of photons in two modes of the same order of magnitude become negligibly small when the number of photons $n+m$ increases. Thus, one can imagine that non-classical correlations introduced by highly occupied states can be easily suppressed or covered by classical correlations introduced, e.g., by noise.

1. *Construction of "sign" observables*

To consider high occupation states on approximately equal footing, one can take inspiration from the qubit case (single-photon subspace). This choice of inspiration for our construction is compeling as for this scenario one can obtain the maximal violation of the CHSH-like inequality using normalized Stokes operators. This is because, as we discussed, in this subspace these operators act exactly like Pauli matrices. In the goal of making new operators in some sense more similar to Pauli matrices for states with higher photon number, one would like to reduce the spectrum of new observables to more closely correspond to the spectrum ± 1. Looking into the action of $\hat{S}_3$ on the qubit states, one can opt to treat in the extended picture states $|n,m\rangle$ with $n>m$ analogusly to qubit state $|0\rangle \equiv |1,0\rangle$ and asign to them eigenvalue 1 and states with $n<m$ as qubits $|1\rangle \equiv |0,1\rangle$ with eigenvalue -1. This is the path that we have chosen in the work [PhD1]. As Stokes operators are first and foremost associated with the analysis of the polarization, let us consider the two modes to be two orthogonal polarization modes, with obvious generalization to any set of two orthogonal modes. Upon presented motivation, we proposed in the article [PhD1] the following observables for the analysis of non-classical behaviour of the states, which we call *sign Stokes operators*:

$$\hat{G}(s) = \text{sign}(\hat{\Theta}(s)) = \text{sign}(\hat{n}_s - \hat{n}_{s_\perp}) = \text{sign}(U_s(\hat{n}_H - \hat{n}_V)U_s^\dagger), \tag{42}$$

where s denotes chosen setting associated with some polarization basis $\{s, s_\perp\}$ and $\hat{n}_s(s\perp)$ stand for the photon number operators in these modes. In the last equation, we introduce the operator $\hat{U}_s$ which denotes a unitary transformation between a linear polarisation basis $\{H,V\}$ and an arbitrary polarisation basis $\{s, s_\perp\}$. This was introduced to intuitively show how one can perform such a measurement, which is completely analogous to the measurement of the Stokes operators. First, one performs a unitary operation on the state that transforms photons with polarization s ($s_\perp$) into photons with polarization H (V). This transformation involves only phase-shifting and polarization rotation transformation, which can be achieved by rotation of the axis of the birefringent crystal used for the analysis of linear polarization. Then this unitary transformation is followed by the photon counting in two output beams from the crystal, i.e., in chosen linear polarization modes $\{H,V\}$. Let us comment that these operators were also independently proposed in the same year and used in the analysis of BEC states [73], however, only in the regime of weakly occupied states. Observe that this construction simplifies the Stokes operators, reducing their spectrum to ± 1, 0. The appearance of additional eigenvalue in comparison to Pauli matrices is a consequence of the fact that states of the form $|n,n\rangle$ do not have an analog in the single-photon subspace.

An important feature of this measurement scheme is the fact that one can use the experimental data to simultaneously analyze the results for all variations of Stokes operators. This is because all of them only make a reassignment of the eigenvalues. However, the sign Stokes operators have an additional property that in fact their expectation value does not depend on the model of the intensity used as long as the intensity value increases with photon number. In other words, one can replace $\hat{n}_s \to \hat{I}_s$ in (42) where $\hat{I}_s$ is some intensity operator that can, for example, describe the detector response and obtain exactly the same prediction. Therefore, one can also use intensity measurements that do not make direct photon counting. It is also important to note, that in fact by making the spectrum of our operators more similar to the spectrum of Pauli matrices, we had to pay a price of loosing another property also associated with Pauli matrices. More precisely, for Stokes operators one can build the Stokes vector $\langle \hat{\vec{\Theta}} \rangle = (\langle \Theta_1 \rangle, \langle \Theta_2 \rangle, \langle \Theta_3 \rangle)$ norm of which is invariant under unitary transformation of basis modes. The analogous statement holds for Pauli operators and normalized Stokes operators. This is, however, not true for sign Stokes operators. This property is crucial in standard derivations of entanglement indicators. Therefore, if one wants to obtain entanglement indicators based on sign Stokes operators different from Bell inequalities, one has to develop new methods for their derivation.

2. Bell inequality violation

Application of the sign function to the Stokes operators effectively performs an alternative normalization of their spectrum, which is crucial to enable the derivation of the Bell inequalities as discussed in Section II C 2. To show that our normalization procedure gives an advantage over normalized Stokes operators, we consider two examples. As a first example, we consider a BSV state. However, for small Γ, this state is dominated by the vacuum contribution to which $\hat{G}(s)$ assigns 0 which prevents observing the violation of a CHSH-like inequality. To cure that, one can modify slightly sign Stokes operators acting on the beam of the X-th party by assigning, for example, eigenvalue -1 to zero photon state:

$$\hat{G}^X(s) \to \hat{G}^{X-}(s) = \hat{G}^X(s) - \hat{\Pi}_{\Omega^X}. \tag{43}$$

Here, operator $\hat{\Pi}_{\Omega^X}$ stands for projector onto the subspace of the Fock space characterized by zero photons in the local beam X. This change preserves the spectrum $\{\pm 1, 0\}$ of these operators. Thus, one can analogously obtain a CHSH-like inequality corresponding to these operators as for the case of normalized Stokes operators discussed in Section II C 2:

$$\begin{aligned} |CHSH_{G-}| = |\langle G^{1-}(1,\lambda)G^{2-}(1,\lambda) + G^{1-}(1,\lambda)G^{2-}(2,\lambda) \\ + G^{1-}(2,\lambda)G^{2-}(1,\lambda) - G^{1-}(2,\lambda)G^{2-}(2,\lambda)\rangle_{LHV}| \leq 2. \end{aligned} \tag{44}$$

Here, $G^{X-}(s,\lambda)$ stands for hypothetical local hidden values of outcomes corresponding to the measurement of the observable $\hat{G}^{X-}(s)$ and the averaging is over a distribution $\rho(\lambda)$. For the analysis, we have chosen the settings used in Section II C 1 which are also optimal for the case of violating the CHSH-like inequality based on normalized Stokes operators using the BSV state. For the second example, we analogously build Mermin-like inequality to examine Bell non-classicality of the BGHZ state:

$$\begin{aligned} |M(3)_{G-}| = |\langle G_1^{1-}(\lambda)G_1^{2-}(\lambda)G_1^{3-}(\lambda) - G_1^{1-}(\lambda)G_2^{2-}(\lambda)G_2^{3-}(\lambda) \\ - G_2^{1-}(\lambda)G_1^{2-}(\lambda)G_2^{3-}(\lambda) - G_2^{1-}(\lambda)G_2^{2-}(\lambda)G_1^{3-}(\lambda)\rangle_{LHV}| \leq 2. \end{aligned} \tag{45}$$

Here, $G_i^{X-}(\lambda)$ represents the local hidden values associated with sign Stokes operators build upon the Stokes operator $\hat{\Theta}_i^X$.

In both cases comparing the results obtained with sign and normalized Stokes operators, we have found that one obtains stronger violation using sign Stokes operators. Importantly, the range of violation in terms of Γ is also broader for the case of the sign Stokes operators. Thus, one can observe with our approach a violation of Bell inequality using states with higher average photon numbers. In the case of BGHZ our analysis was restricted to $\Gamma < 0.9$ due to the limitations of the approximation method used to calculate the probability amplitudes. However, we find that there is a violation in the entire analyzed range of Γ for sign Stokes operators, while for normalized Stokes operators, violation is already no longer present for $\Gamma > 0.77$. For the BSV state, the range of violation increases with the cut-off of the maximal number of photons in (14) used in numerical calculations. Therefore, we conjecture that the violation is present for any Γ. In the supplementary material, we have provided strong motivation for this conjecture, based on an analysis of patterns of violation by different terms $|\psi_-^n\rangle$ of (14). Assuming conservation of observed patterns, one can show that the quantum expectation value of CHSH-like expression for sign Stokes operators is lower bounded by 2 with the bound reached in the limit $\Gamma \to \infty$. Therefore, one can conjecture that theoretically sign Stokes operators reveal Bell non-classicality of states with an arbitrarily high average number of photons. From a more experimental perspective, we analyzed the robustness of the violation against uncorrelated noise and inefficient detectors. In the result, we found that also in this case sign Stokes operators achieve a significant advantage over the normalized variant. Therefore, sign Stokes operators provide a highly improved measurement scheme for revealing Bell non-classicality of states of quantum optical fields with undefined photon numbers.

C. Contextuality with quantum bosonic fields

The incompatibility of quantum mechanics with non-contextual hidden variable models is an active field of research that is motivated by its potential importance for speedup in quantum computations [66, 67]. Similarly, as in the case of Bell inequalities, the majority of the research was conducted concerning finite-dimensional systems with a definite number of particles. Therefore, scenarios based on states with undefined particle numbers are still not well examined. In addition, efforts in this matter were concentrated on the continuous variable regime [74, 75]. Therefore, one of the main goals of our article [PhD2] was to analyze the contextuality using states of quantum bosonic fields with undefined number of particles in the discrete variable regime. We propose a new representation of $\mathfrak{su}(2)$ on two-mode Fock space that allowed us to construct a generalization of the Peres-Mermin square for quantum bosonic fields.

1. Construction of Pauli-like operators for bosonic fields

As the Peres-Mermin square is based on Pauli matrices, its generalization could be done if one would find their counterparts for the bosonic Fock space. One could think of the Stokes operators as a good candidate, as they provide a $\mathfrak{su}(2)$ representation similarly to Pauli matrices. However, this is insufficient. This is because in the construction of the Peres-Mermin square, the anticommutation relations play an important role, and they are not fulfilled by Stokes operators. Also, the unbounded nature of these operators as discussed for Bell inequalities can cause problems when dealing with hidden variable models. However, a simple spectrum reduction, as in the case of sign Stokes operators can cause a loss of properties associated with $\mathfrak{su}(2)$.

To address these problems we propose the following set of operators as the counterpart of Pauli matrices in the two-mode Fock space:

$$\begin{aligned} \hat{\mathcal{G}}_0 &= \mathbb{1} - \textstyle\sum_n |n,n\rangle\langle n,n|, \\ \hat{\mathcal{G}}_1 &= \textstyle\sum_{n\neq m} |n,m\rangle\langle m,n|, \\ \hat{\mathcal{G}}_2 &= -i\,\mathrm{sign}(\hat{a}^\dagger\hat{a} - \hat{a}_\perp^\dagger\hat{a}_\perp)\textstyle\sum_{n\neq m} |n,m\rangle\langle m,n|, \\ \hat{\mathcal{G}}_3 &= \mathrm{sign}(\hat{a}^\dagger\hat{a} - \hat{a}_\perp^\dagger\hat{a}_\perp), \end{aligned} \tag{46}$$

where $\mathbb{1}$ stands for the identity on two modes. This set is proposed in such a way that it mimics the action of Pauli matrices on states $|n,m\rangle$ with the association of states with $n > m$ to $|0\rangle$ and $n < m$ to $|1\rangle$. As required for operators associated with the representation of the $\mathfrak{su}(2)$ algebra, these operators satisfy the identical commutation relation as those of the Pauli matrices:

$$[\hat{\mathcal{G}}_i, \hat{\mathcal{G}}_j] = 2i\epsilon_{ijk}\hat{\mathcal{G}}_k, \tag{47}$$

where $i,j,k = 1,2,3$. This is also the case with the anticommutation relation:

$$\{\hat{\mathcal{G}}_i, \hat{\mathcal{G}}_j\} = 2\delta_{ij}\hat{\mathcal{G}}_0. \tag{48}$$

These relations result in the crucial for Peres-Mermin square relation:

$$\hat{\mathcal{G}}_i\hat{\mathcal{G}}_j = \delta_{ij}\hat{\mathcal{G}}_0 + i\epsilon_{ijk}\hat{\mathcal{G}}_k. \tag{49}$$

Furthermore, the $\hat{\mathcal{G}}_0$ operator commutes with all $\hat{\mathcal{G}}_i$ operators and plays the role of the counterpart to the identity $\hat{\sigma}_0 = \mathbb{1}_2$ on the qubit space. Let us stress a pitfall of our construction. In our work, we do not propose the experimental realization of the measurement corresponding to the operators $\hat{\mathcal{G}}_1$ and $\hat{\mathcal{G}}_2$. Therefore, this poses an open problem for the development of such a technique outside of the theoretical realm. Note further that the set (46) is not equivalent to operators $\hat{G}_s$, with $s = 1,2,3$ standing for three maximally unbiased polarization bases.

2. Generalization of the Peres-Mermin square

Using our Pauli-like operators, we propose a version of the Peres-Mermin square suitable for the 2×2 mode states of quantum bosonic fields. We do so by mapping the original Peres-Mermin square (see Section II D) as follows: $\hat{\sigma}_i^1 \otimes \hat{\sigma}_j^2 \to \hat{\mathcal{G}}_i^1 \hat{\mathcal{G}}_j^2$. Using the convention of notation of Section II D we denote elements of the Peres-Mermin square by $\hat{A}_{ij}$. The relation (49) ensures that one can find the analogous sets of compatible observables as the ones for the two-qubit case (sets of operators $\hat{A}_{ij}$ with one shared index).

To analyze the problem of contextuality consider operator:

$$\begin{aligned} \hat{O} = \hat{A}_{11}\hat{A}_{12}\hat{A}_{13} + \hat{A}_{21}\hat{A}_{22}\hat{A}_{23} + \hat{A}_{31}\hat{A}_{32}\hat{A}_{33} \\ +\hat{A}_{11}\hat{A}_{21}\hat{A}_{31} + \hat{A}_{12}\hat{A}_{22}\hat{A}_{32} - \hat{A}_{13}\hat{A}_{23}\hat{A}_{33}, \end{aligned} \tag{50}$$

where, in each term, is either poroduct of the elements of a column or row of the generalized Peres-Mermin square. With this operator, one can formulate an inequality that has to be fulfilled by non-contextual hidden variable (NCHV) models. The procedure of obtaining the bounds for the NCHV models [76] is, in fact, analogous to obtaining the bounds for Bell inequalities for LHV models presented in the Section II C 1. Although our Pauli-like observables have a different spectrum than Pauli matrices, i.e., $\pm 1, 0$, one obtains the same non-contextual bound for our observable as for the case for an analogous if one would build the operator (50) with the original Peres-Mermin square. The obtained inequality reads:

$$\begin{aligned} \langle A_{11}A_{12}A_{13} + A_{21}A_{22}A_{23} + A_{31}A_{32}A_{33} \\ +A_{11}A_{21}A_{31} + A_{12}A_{22}A_{32} - A_{13}A_{23}A_{33}\rangle_{NCHV} \leq 4, \end{aligned} \tag{51}$$

where A_{ij} stand for hidden values corresponding to outcomes of measurement of observables $\hat{A}_{ij}$.

Now concerning quantum predictions, one can find that $\hat{O} = 6\hat{\mathcal{G}}_0^1\hat{\mathcal{G}}_0^2$ as the first five terms of (50) are all equal to $\hat{\mathcal{G}}_0^1\hat{\mathcal{G}}_0^2$ while the last term is equal to $-\hat{\mathcal{G}}_0^1\hat{\mathcal{G}}_0^2$. Observe that the operator $\hat{\mathcal{G}}_0^1\hat{\mathcal{G}}_0^2$ is a projection into the subspace of the Fock space spanned by states $|k,l;n,m\rangle$ with $k \neq l$ and $n \neq m$. Therefore, for a state $\hat{\rho}$ the expectation value of operator $\hat{O}$ is given by:

$$\langle \hat{O} \rangle_\rho = 6 - 6P(k = l \vee n = m|\rho), \tag{52}$$

where $P(k = l \vee n = m|\rho)$ stands for the probability for the state ρ of detecting the same number of particles in both modes of at least one of the parties. Clearly, whenever $P(k = l \vee n = m|\psi) < \frac{1}{3}$ the inequality (51) is violated and the contextuality is revealed.

Let us comment that whenever one considers states with a single photon per party (two optical qubits), one retrieves the original Peres-Mermin square for which on has $\langle \hat{O} \rangle_\rho = 6$ for any state. Note that this state-independence is lost in general in our approach. However, one could argue that approximately one regains state-independence in the regime of a high average number of photons. To see this, first consider two modes. For each set number of particles n shared between the modes, there is either 0 (odd n) or 1 (even n) Fock state which has the same number of particles in both modes. Therefore, with increasing n, the ratio between the Fock states with equal and unequal number of particles converges to 0. Based on this discussion, it is clear that also in the four-mode case the Fock states with equal number of particles in modes of at least one party (only those can contribute to $P(k = l \vee n = m|\rho)$) also form a minority when a high particle number in both parties is considered. Therefore, if there is no specific mechanism that favors states from this minority class, their contribution in most cases will diminish in high occupations states, and one will have in general $\langle \hat{O} \rangle_\rho \approx 6$. A primary example of such a mechanism that favors these specific states is the interaction corresponding to two-mode squeezing or its generalization into more modes. Such interactions originating from non-linearities are rather weak, and naturally occurring high occupation states rarely have their origin in such processes. Still, even if two-mode squeezing is present (being a dominant process in state preparation), one could reveal contextuality based on resulting states by choosing different partition of modes into subsystems, as it is the case, e.g., with the BSV state. Figure

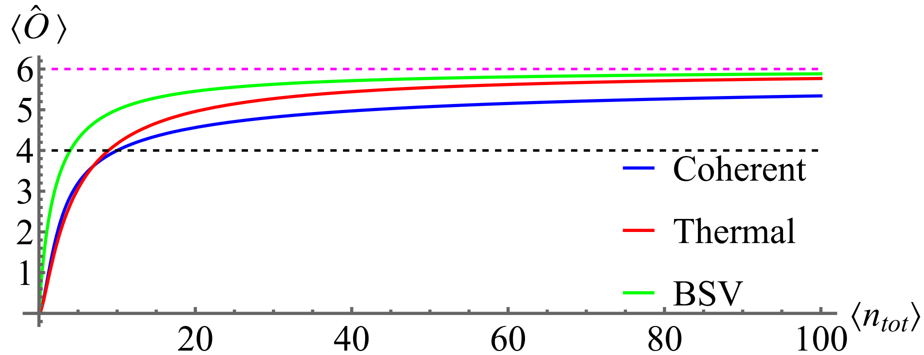

FIG. 1. Quantum expectation value $\langle \hat{O} \rangle$ as a function of average total number of particles $\langle n_{tot} \rangle$ (51) for BSV, four mode coherent and thermal state. Magenta dashed line denotes quantum bound and black dashed line denotes NCHV model bound. In the paper [PhD2] only the plot for BSV is given.

1 considers three examples of described behaviour. First, for the BSV state, second, for the Gibbs thermal state of four non-interacting modes, and third example for four modes in coherent states with the same amplitude. Note that, as expected, in all three cases $\langle \hat{O} \rangle$ converges to 6 with an increasing total average number of particles $\langle n_{tot} \rangle$.

3. *Different types of non-classicality*

The proposed Pauli-like operators can be also used to reveal entanglement and Bell non-classicality. One can derive Bell inequalities exactly in the same way as for the normalized and sign Stokes operators. For the entanglement, one finds that the proposed operators admit the mapping of entanglement indicators analogous to Stokes operators. More precisely, having an entanglement indicator written in terms of Pauli matrices, one obtains the entanglement indicator for the quantum bosonic field by mapping $\sigma_i^X \rightarrow \hat{\mathcal{G}}_i^X$. Based on the examined example of BGHZ state we observe an interesting property of the used non-classicality criteria that one approaches the quantum bounds in the limits of high average particle numbers. This is completely opposite to the other approaches, as, for example, normalized Stokes operators. More precisely in such scenarios one is closest to quantum bounds for a small number of particles and from some point observed non-classical behaviour diminishes with an increasing number of particles, and this is something that one would normally not expect.

D. Generalization of Gisin's theorem to quantum fields

One of the fundamental results in quantum mechanics is Gisin's theorem. It answers the question of whether entanglement of pure states is always connected with Bell non-clasicality. The first version for two-particles by Gisin [77] was then developed [78–81] to state that for each pure entangled state of the system containing an arbitrary number of particles with arbitrary dimensions of single-particle spaces, there exists a Bell inequality violated by this state. However, this does not give a final answer to the problem, as the analysis of the problem was carried out within the first quantization, which requires fixing the number of particles considered. This therefore does not cover all scenarios in quantum field theory in which one can deal with entangled states with an undefined number of particles such as, e.g., the BSV state. In the article [PhD3] we extend Gisin's theorem to cover this case.

1. *Outline of the proof*

First we introduce a crucial tool for our proof of Gisin's thoerem for quantum fields. This tool is a field Schmidt decomposition in the Fock space. Note that from the construction, the Fock space has no tensor product structure which allows the standard Schmidt decomposition. Therefore, to construct Schmidt decomposition we first divide the modes of the field into two families $\{a_i\}$, and $\{b_l\}$ (here i and l are countable indices). The families have the property for bosons $[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}$, $[\hat{b}_i, \hat{b}_j^\dagger] = \delta_{ij}$ $[\hat{a}_i, \hat{b}_l^\dagger] = 0$ and an anti-commutator version of these holding in the fermionic case. One might think of modes $\{a_i\}$ and $\{b_l\}$ as, e.g., spatially separated. Now, each Fock basis state can be associated with two vectors $\vec{n}^j = (n_1^j, n_2^j, ...)$ and $\vec{m}^{j'} = (m_1^{j'}, m_2^{j'}, ...)$ for which the following relations are fulfilled $\sum_{i=1}^{\overline{\{a_i\}}} n_i^j < \infty$, $\sum_{l=1}^{\overline{\{b_l\}}} m_l^{j'} < \infty$. These vectors describe the distributions of a finite number of particles among two groups of orthogonal modes $\{a_i\}$ and $\{b_l\}$. Each Fock state for the selected modes, either bosonic or fermionic, can then be written as

$$\left|\vec{n}^j; \vec{m}^{j'}\right\rangle = \frac{1}{\mathcal{N}_a \mathcal{N}_b} \prod_i (\hat{a}_i^\dagger)^{n_i^j} \prod_l (\hat{b}_l^\dagger)^{m_l^{j'}} |\Omega\rangle = f(\{a_i^\dagger\}, j) g(\{b_l^\dagger\}, j') |\Omega\rangle, \tag{53}$$

where $\mathcal{N}_{a(b)}$ stand for a normalization factor, and $f(\{a_i^\dagger\}, j)$ denote a specific monomial of creation operators in modes $\{a_i\}$ and analogously $g(\{b_l^\dagger\}, j')$ for modes $\{b_l\}$. Importantly, the set $\{\left|\vec{n}^j; \vec{m}^{j'}\right\rangle\}_{jj'}$, indexed by two countable indices j, j', is a countable orthonomal basis in the Fock space considered.

Let us consider two Hilbert spaces $\mathcal{H}_A$, $\mathcal{H}_B$ spanned respectively by abstract orthogonal basis vectors $\tilde{f}(j)$, $\tilde{g}(j')$ with indices j, j' shared with elements of the set $\{\left|\vec{n}^j; \vec{m}^{j'}\right\rangle\}_{jj'}$. Then the linear map:

$$f(\{a_i^\dagger\}, j) g(\{b_l^\dagger\}, j') |\Omega\rangle \mapsto \tilde{f}(j) \otimes \tilde{g}(j'), \tag{54}$$

is an isomorphism between the the considered Fock space and $\mathcal{H}_\mathcal{A} \otimes \mathcal{H}_\mathcal{B}$. One can now map any pure state from Fock space into state in $\mathcal{H}_\mathcal{A} \otimes \mathcal{H}_\mathcal{B}$, which can then be decomposed with standard Schmidt decomposition. By then mapping this state back into Fock space, one arrives in the Schmidt-decomposed form of the original state:

$$|\psi\rangle = \sum_t \lambda_t F(\{a_i^\dagger\}, t) G(\{b_l^\dagger\}, t) |\Omega\rangle, \tag{55}$$

where λ_t are Schmidt coefficients resulting from (1) and $F(\{a_i^\dagger\}, t)$, $G(\{b_l^\dagger\}, t)$ stand for polynomials of creation operators in corresponding groups of modes $\{a_i\}$, $\{b_l\}$. These polynomials fulfill the local orthogonality relation given by:

$$\langle\Omega| F(\{a_i^\dagger\}, t)^\dagger F(\{a_i^\dagger\}, t') |\Omega\rangle = \langle\Omega| G(\{b_l^\dagger\}, t)^\dagger G(\{b_l^\dagger\}, t') |\Omega\rangle = \delta_{t,t'}. \tag{56}$$

What is important is that the uniqueness of the decomposition is preserved. This is up to the local choice of phase factors for polynomials $F(\{a_i^\dagger\}, t)$, $G(\{b_l^\dagger\}, t)$, which, however, results in a unique polynomial $F(\{a_i^\dagger\}, t) G(\{b_l^\dagger\}, t)$.

Based on the Schmidt decomposition and the definition of separability (6) one can observe that any mode entangled state $|\psi_{ent}\rangle$ can be put in the form:

$$\begin{aligned} |\psi_{ent}\rangle = \lambda_1 F(\{a_i^\dagger\}, 1) G(\{b_l^\dagger\}, 1) |\Omega\rangle + \lambda_2 F(\{a_i^\dagger\}, 2) G(\{b_l^\dagger\}, 2) |\Omega\rangle + \lambda_R |R\rangle \\ = \sqrt{|\lambda_1|^2 + |\lambda_2|^2} |\phi_{12}\rangle + \lambda_R |R\rangle, \end{aligned} \tag{57}$$

where $\lambda_1, \lambda_2 \neq 0$ and $|R\rangle$ stands for state emerging from the rest of the terms in Schmidt decomposition, i.e., for $t > 2$, and λ_R is the amplitude corresponding to this state, which can be zero.

One can think of the state $|\phi_{12}\rangle$ emerging from the first two terms as a state in some 2×2 dimensional (two-qubit) subspace. Note that the state $|\phi_{12}\rangle$ is clearly entangled within the considered subspace. From original Gisin's theorem there exists a CHSH inequality which is violated on the positive side by such two-qubit state. Due to the correspondence of the CHSH inequality with the CH inequality for qubits (30) there is also a CH inequality which is violated on the positive side by such a state. One can now construct the Bell operator corresponding to this CH inequality and embed it properly in the Fock space. Let us denote it by $\hat{CH}$. By construction, one has: $\langle \hat{CH} \rangle_{\phi_{12}} > 0$. However, we need to find the violation in the context of the full state $|\psi_{ent}\rangle$. One can use the following: for any operator $\hat{O}$ that acts non-trivially on the considered subspace but assigns eigenvalue 0 to all states from its orthogonal complement, one has that its expectation value is given by:

$$\langle \hat{O} \rangle_{\psi_{ent}} = (|\lambda_1|^2 + |\lambda_2|^2)\langle \hat{O} \rangle_{\phi_{12}} + |\lambda_R|^2 \langle \hat{O} \rangle_R = (|\lambda_1|^2 + |\lambda_2|^2)\langle \hat{O} \rangle_{\phi_{12}}. \tag{58}$$

Here in the second equality, the second term disappears as $|R\rangle$ is a state from the orthogonal complement of the considered subspace. As this operator is constructed based on projectors into the considered 2×2 dimensional subspace or its local parts, it fulfills the relation (58). Thus, we finally get:

$$\langle \hat{CH} \rangle_{\psi_{ent}} = (|\lambda_1|^2 + |\lambda_2|^2)\langle \hat{CH} \rangle_{\phi_{12}} > 0, \tag{59}$$

what indicates violation of the CH inequality for the state $|\psi_{ent}\rangle$. Therefore, we showed that Gisin's theorem holds also for any pure mode-entangled states of a single quantum field. Generalization to any finite number of distinguishable fields is straightforward.

2. *Further application of Schmidt decomposition in the Fock space*

The Schmidt decomposition in Fock space can be used as a tool in designing experimental setups that reveal non-classical effects based on entanglement. In particular, it provides a sufficient condition for the necessity of using ancillary resources for experimental revealing of non-classicality of entangled states. These resources could be, for example, coherent states in ancillary modes.

Consider a state $|\psi\rangle$. One is not able to reveal non-classicality originating from entanglement of this state using passive optics if all projections of the state $|\psi\rangle$ into the subspace given by $\sum_i n_i = n$, $\sum_{i'} m_{i'} = m$, i.e., with set number of particles for each party, have Schmidt rank 1, that is:

$$\forall_{n,m} \frac{1}{N} \Pi_{nm} |\psi\rangle = F^n(\{a_i^\dagger\}, 1) G^m(\{b_l^\dagger\}, 1) |\Omega\rangle \,. \tag{60}$$

Here N stands for a normalization factor, Π_{nm} denotes a projector onto the subspace with n and m particles in first and second party respectively, and $F^n(\{a_i^\dagger\}, 1)$, $G^m(\{b_l^\dagger\}, 1)$ are polynomials of creation operators that have terms that are only of order n, m in creation operators respectively.

The primary reason for such a condition appearing is the fact that currently realizable measurements do not allow direct measurements of projections into states such as $(|n\rangle + |m\rangle)/\sqrt{2}$. All experimentally realizable measurements at the end simply consist of some intensity (particle number) measurement in some modes. Thus, one has to be able to reduce the problem into such a measurement. Whenever criterion (60) is fulfilled, one is unable to propose a measurement of this kind that would reveal entanglement-based effects without additional resources (modifications to the setup). This is because the expectation value of any observable that can be written solely using projections into Fock states (this is the case for perfect photo-detection) is a weighted average over the expectation values of this observable for states $\frac{1}{N}\Pi_{nm} |\psi\rangle$. In the case considered, all $\frac{1}{N}\Pi_{nm} |\psi\rangle$ are separable; thus, any criterion based on such observables will not show entanglement. However, by adding ancillary modes $\{c_i^\dagger\}$ in a suitable state, one might find that the modified state $|\psi + ancila\rangle = f_a(\{c_i^\dagger\}) |\psi\rangle$, where $f_a(\{c_i^\dagger\})$ stands for a polynomial of creation operators in ancillary modes, does not satisfy the condition (60), when written in terms of final modes (essentially, the ones observed by the detectors). Then it might be possible to reveal the entanglement of such a state using photo-detection. In fact, if this is not the case, one knows that the ancillary system was not designed properly for the given problem.

Note that, ancilla is not formally entangled with modes constituting $|\psi\rangle$. Still, to ensure that non-classicality emerges, the ancilla photons must be indistinguishable with the "signal" photons from the original state $|\psi\rangle$. Of course, if this indistinguishably is not perfect, the entanglement effect persists if this imperfection is small, up to a certain threshold.

E. Open dynamics of entanglement in mesoscopic bosonic fields

Simplifying the description of quantum systems is of great importance in the perspective of scaling up the system size under theoretical considerations to mesoscopic scales. This is of particular interest in the context of scaling up quantum technologies. Such simplifications require one to choose only part of the degrees of freedom to be relevant for the given study and dismiss the others from the analysis. However, to obtain a coherent framework, one has to additionally ensure that the remaining information about degrees of freedom is sufficient to allow a sensible description of their evolution. In this matter, one is among other things interested in describing decoherence effects imposed by the interaction with the environment which results in open evolution.

Bosonic quantum systems are of interest from the quantum information perspective, as they can potentially find applications in both the cybersecurity sector and quantum computing. Let us recall that recently an easy and intuitive mesoscopic description of such systems was proposed, that is, the reduced state of the field formalism (RSF) [69]. However, it has the caveat that one is unable to access information about entanglement within this framework. Because entanglement is crucial for quantum information tasks in article [PhD4] we propose an extension of the RSF formalism to adapt it to the description of this quantum phenomenon.

F. Construction of the extended reduced state of the field formalism

In the simplest form our extended RSF framework consists of two structures: the single particle density matrix from the original formulation, and extended reduced state:

$$\hat{\rho} = \sum_{k,k'=1}^{N} \mathrm{tr}\Big\{\hat{\rho}_F \hat{a}^\dagger_{k'} \hat{a}_k\Big\} |k\rangle \langle k'| \,, \tag{61}$$

$$\hat{\rho}_4 := \sum_{k,k',n,n'}^{N} \mathrm{tr}\Big\{\hat{\rho}_F \hat{a}^\dagger_{n'} \hat{a}_n \hat{a}^\dagger_{k'} \hat{a}_k\Big\} |n,k\rangle \langle n',k'| \,. \tag{62}$$

The extended reduced state follows the convention of assigning kets to annihilation operators and bras to creation operators in the matrix elements, i.e., expectation values. Clearly, this structure keeps information about all particle number correlations in the state. In previous sections, the important role of such correlations from the perspective of detecting non-classical phenomena was already marked. The introduction of the extended reduced state $\hat{\rho}_4$ allows one to consider in the analysis an additional class of observables that are reduced in analogy to (35):

$$\hat{O}_4 = \sum_{n,n',k,k'} o_{n',n,k',k} \hat{a}^\dagger_{n'} \hat{a}_n \hat{a}^\dagger_{k'} \hat{a}_k \to \hat{o}_4 = \sum_{n,n',k,k'} o_{n',n,k',k} |n',k'\rangle \langle n,k| \,. \tag{63}$$

This reduction also preserves expectation values in the sense $\mathrm{tr}\Big\{\hat{\rho}_F \hat{O}_4\Big\} = \mathrm{tr}\{\hat{\rho}_4 \hat{o}_4\}$.

In addition, an important feature of this extension is the fact that the evolution equation can be derived for $\hat{\rho}_4$ which corresponds to (37) . We shall present here the equation for the case of no coherent pumping.

This equation for Markovian open evolution reads:

$$\begin{aligned}\frac{d}{dt}\hat{\rho}_4 = &-\frac{i}{\hbar}[\hat{h}\otimes\mathbf{1}+\mathbf{1}\otimes\hat{h},\hat{\rho}_4]+\sum_j \kappa_j(\hat{u}_j\otimes\hat{u}_j\hat{\rho}_4\hat{u}_j^\dagger\otimes\hat{u}_j^\dagger-\hat{\rho}_4)\\ &+\frac{1}{2}\{(\mathbf{1}\otimes\hat{\gamma}_\uparrow+\hat{\gamma}_\uparrow\otimes\mathbf{1})-(\mathbf{1}\otimes\hat{\gamma}_\downarrow^T+\hat{\gamma}_\downarrow^T\otimes\mathbf{1}),\hat{\rho}_4\}\\ &+(\hat{\rho}\otimes\gamma_\downarrow^T)^{\tau_L}+(\gamma_\uparrow\otimes\hat{\rho})^{\tau_L}+\gamma_\uparrow\otimes\hat{\rho}+\hat{\rho}\otimes\gamma_\uparrow+(\gamma_\uparrow\otimes\mathbf{1})^{\tau_L},\end{aligned} \tag{64}$$

with $\tau_L : |n,m\rangle \to |m,n\rangle$ and $\hat{h},\hat{\gamma}_\updownarrow,\hat{u}_j$ as in (38) . To solve this equation one clearly first has to find the time evolution of the $\hat{\rho}$. Therefore, to use this equation, one has to first consider the evolution equation of the original RSF formalism (38). Here, the first Heisenberg-like term corresponds to the unitary evolution of the system. The second term describes random unitary scattering, and the remaining terms are responsible for dissipation or incoherent pumping from the environment. Note that, one can also include coherent pumping in two ways. One can either add additional structures to the formalism (see [PhD4]) or consider an additional mode in the coherent state and linearly couple it to the pumped mode.

Note that $\hat{\rho}_4$ is in general not Hermitian, contrary to $\hat{\rho}$ and thus has no state-like properties. However, to consider entanglement, one has to first choose the bipartition of modes. To do so, two sets of indices can be chosen that correspond to the modes and determine the subsystems $\mathcal{I}_A,\mathcal{I}_B$ with $\mathcal{I}_A\cap\mathcal{I}_B=\varnothing$. Given this selection, one can apply the following projection to the operator $\hat{\rho}_4$:

$$\hat{\rho}_4 \to \hat{\rho}^{\Pi} := \hat{\Pi}_{\mathcal{I}_A,\mathcal{I}_B}\hat{\rho}_4\hat{\Pi}_{\mathcal{I}_A,\mathcal{I}_B} = \sum_{i,n\in\mathcal{I}_A}\sum_{j,m\in\mathcal{I}_B}\rho_{ijnm}\,|i,j\rangle\langle n,m|\,, \tag{65}$$

where $\rho_{ijnm}=\langle\hat{a}_n^\dagger\hat{a}_i\hat{a}_m^\dagger\hat{a}_j\rangle$ and

$$\Pi_{\mathcal{I}_A,\mathcal{I}_B} = \sum_{i\in\mathcal{I}_A}\sum_{j\in\mathcal{I}_B}|i,j\rangle\langle i,j|\,. \tag{66}$$

One can find that $\hat{\rho}^{\Pi}$ after normalization possesses all the mathematical properties of a density matrix of two qudits. The dimension of each qudit is determined by the number of modes in a given party. This could be seen as a density matrix on the two-particle-like Hilbert space constructed as the tensor product of single-particle-like Hilbert spaces for considered subsystems used in the original RSF. This makes a direct connection between our extended formalism and the original RSF approach. It is important that, while $\hat{\rho}^{\Pi}$ and $\hat{\rho}$ have state-like properties, they do not inherit probabilistic interpretation associated with the states. Here, the diagonal elements of $\hat{\rho}^{\Pi}$ instead of probabilities describe the correlation of particle numbers between modes. Let us comment that whenever evolution does not couple modes between the parties, one can directly consider evolution of $\hat{\rho}^{\Pi}$ instead of full $\hat{\rho}_4$.

1. *Entanglement within extended reduced state of the field formalism*

The important aspect is how one can examine entanglement within the extended RSF formalism. Crucial for this aspect is the fact that whenever the reduced two-particle-like state $\hat{\rho}^{\Pi}$ is entangled, the original state of the field $\hat{\rho}_F$ is also entangled. In other words, the entanglement of $\hat{\rho}^{\Pi}$ is a sufficient criterion for the entanglement of $\hat{\rho}_F$. The proof of this statement is based on the proof of the mapping of entanglement indicators for Stokes operators [42] or Pauli-like operators $\hat{\mathcal{G}}_i$ [PhD2]. Due to this result, one can simply apply any method of revealing the entanglement for two qudits to $\hat{\rho}^{\Pi}$. In the case two-qubits, i.e., four modes , one can use the PPT criterion [82] for the entanglement which is sufficient and necessary. Therefore, in such a scenario, if one does not reveal the entanglement, then the state $\hat{\rho}^{\Pi}$ does not contain information about it. However, this does not indicate that $\hat{\rho}_F$ is necessarily separable. Observe that to apply this methodology, one has to have at least four modes. However, one can also reveal the entanglement of two-mode states by proper extension of the state to four modes. An example of such an extension is to take the state of two additional modes as a copy of the original state $\hat{\rho}_F$.

In the article we consider an example of entangled Gaussian state (BSV) , and non-Gaussian state of the single photon which was symmetrically beam-splitted into two modes. In both cases, our methodology allows for detecting entanglement. Furthermore, for the BSV state we find that $\hat{\rho}^{\Pi}$ allows detecting entanglement for any finite amplification gain Γ (see (14)), that is, for any average number of photons characterizing the state. Then analysis of the time evolution imposed on these states by thermal environment allowed us to show that entanglement for both these states is robust against low-temperature damping. What is more, we observed that for the BSV state limit of amplification gain $\Gamma \to \infty$ provides the longest time for which $\hat{\rho}^{\Pi}$ shows entanglement. This is for any temperature of the thermal bath.

2. *Other types of non-classicality*

The extended RSF can also be used in the description of another type of non-classicality. In particular, one can consider the quantum effect of sub-Poissonian statistics and its connections to entanglement. In this matter, we consider a generalization of the Mandel Q parameter:

$$\mathcal{Q}_{ij} := \frac{\langle \hat{a}_i^\dagger \hat{a}_j \hat{a}_j^\dagger \hat{a}_i \rangle - \langle \hat{a}_i^\dagger \hat{a}_j \rangle \langle \hat{a}_j^\dagger \hat{a}_i \rangle}{\langle \hat{a}_i^\dagger \hat{a}_i \rangle} - 1 < 0, \tag{67}$$

where whenever inequality holds one finds quantum phenomenon. For $i = j$ one has the normal Mandel Q parameter, the negativity of which indicates sub-Poissonian statistics. When $i \neq j$ negative value of this parameter indicates entanglement. Then using tools of the extended RSF formalism, we showed the relation between the entanglement created by beam splitting a single occupied mode into two modes and sub-Poissonian statistics of the input mode:

$$\mathcal{Q}_{12}^{out} + \mathcal{Q}_{21}^{out} = \mathcal{Q}_{11}^{in}. \tag{68}$$

Here, we assume that the input mode a_1 is occupied and the superscripts denote whether the parameter $\mathcal{Q}_{ij}$ is calculated for the input or output modes of the beamsplitter. From this relation, one clearly sees how sub-Poissonian statistics is directly transformed into entanglement.

Finally, let us make a comment that contrary to the analysis of entanglement, it is not sufficient to keep only ρ^{Π} to consider sub-Poissonian statistics. For such an analysis, one needs the full ρ_4. This is an additional reason for the formulation of the extended RSF using ρ_4.

IV. PERSPECTIVES FOR FURTHER RESEARCH

The presented research focused on providing tools for describing non-classical phenomena of states with an undefined particle number. What is more, the special emphasis was put on the regime with high average particle number. The results show that quantum field theory predicts the non-classical behavior of states also on such scales. Going outside of such fundamental considerations towards a more pragmatic approach, the question arises whether there are quantum information tasks where such states could give some kind of an advantage. In relation to this question one might ask if the proposed measurement scheme given by sign Stokes operators could be used in some device-independent quantum cryptography protocol, and what would be the pros and cons of such an approach. This is a promising avenue, as violation of Bell inequalities using this measurement scheme is more robust against noise and losses than for previous approaches in the context of states with an undefined number of particles.

Furthermore, while the experimental realization of sign Stokes operators is conceptually straightforward, this is not the case for proposed Pauli-like operators. As these operators work extremely well in revealing the non-classiclaity of states with a high average number of photons, at least in the examined cases, it is an interesting problem to propose some experimental realization of such operators.

The extended reduced state of the field framework also opens multiple paths for further development. For example, one can try to perform a classification of states based on its mesoscopic properties in terms of reduced states and of the role of these properties for quantum information tasks. Furthermore, this formalism allows for easy analysis of open dynamics of,e.g., different quantum optical setups, by specifying mesoscopic properties of the sources. This is possible because, among other things, one can easily include passive optical elements into the framework. What is more, one can consider what other non-classical phenomena could be described using this formalism. One such example could be higher-order polarization, sometimes called hidden polarization [83], as one could use this formalism to consider second-order polarization tensors. The first quantization-like structure associated with the formalism allows for using multiple tools from quantum mechanics. Thus, one can look for the tools that can be applied to the reduced state with the results that have a useful interpretation in the context of the full state of the field, as in the case of the PPT criterion and entanglement.

Further, one can still look for new tools for detecting the quantumness of states with an undefined number of particles in highly occupied regimes. On the one hand, this can be done in the sense of finding more robust measurement schemes. On the other hand, one can consider methods of detecting different types of non-classicality for such states like, for example, steering.

Finally, going back fully to fundamental questions, it is an interesting topic how the connection between entanglement and Bell non-classicality translates into theories which concern curved spacetimes. This problem is non-trivial, as for example the concept of a particle is in general not well defined in the quantum field theory in curved (classical) spacetime [84]. There could also be differences in the predictions between when one considers quantum theory of gravity like loop quantum gravity or when one assumes classical spacetime.

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Simplified quantum optical Stokes observables and Bell's theorem

Konrad Schlichtholz✉, Bianka Woloncewicz✉ & Marek Żukowski

We discuss a simplified form of Stokes operators for quantum optical fields that involve the known concept of binning. Behind polarization analyzer photon numbers (more generally intensities) are measured. We have two outputs, say, for horizontal and vertical polarization. If the value obtained in horizontal output is greater than in vertical one we put 1. Otherwise, we put – 1. For equal photon numbers, we put 0. Such observables do not have all properties of the Stokes operators, but can be employed in Bell type measurements, involving polarization analyzers. They are especially handy for states of undefined number of photons, e.g. squeezed vacuum and their realisation is intuitive. We show that our observables can lead to quite robust violations of associated Bell inequalities. We formulate a strongly supported numerically conjecture that one can observe with this approach violations of local realism for the four mode squeezed vacuum for all pumping powers (i.e. gain values).

The discussion about what is the essence of quantumness started with the first attempts of formulating quantum mechanics. With the emblematic paper of Einstein et al.[1] the problem of completeness of quantum mechanics became a point of discussion among the scientific community. This started with the response by Bohr[2]. Many years later, after the paper of Bell[3] the challenge of revealing non-classicality, in terms of violation of local realism, has entered the core of contemporary research. All that in the meantime gained in importance with the emergence of quantum information and communication.

The ultimate test of non-classicality is the violation of Bell inequalities. This is now also the essence of testing of device-independent quantum communication protocols. Formulations of Bell's theorem for situations of fixed numbers of particles have already a vast literature, and well established methods, see e.g. reviews[4–7]. However, if one moves to situations with undefined numbers of particles, still the situation is quite open. This is of course e.g. the case of general quantum optical fields. A lot of approaches are tested.

Polarization entanglement experiments are classic examples of experimental tests of Bell's inequalities. The two photon experiments are a realization of two qubit-entanglement[8,9]. A deceptively obvious step in the direction towards optical fields of undefined photon numbers is to use quantum Stokes observables. The usual definition of these runs as follows. If one assumes that the intensity of light is proportional to the photon number, then (standard) quantum Stokes observables are given by $\hat{\Theta}_i = \hat{a}^{\dagger}{}_i\hat{a}_i - \hat{a}^{\dagger}{}_{i\perp}\hat{a}_{i_\perp}$, where $\hat{a}$ is an annihilation operator. Indices $i = 1, 2, 3$ mark three mutually unbiased (fully complementary) polarization analyzers settings. The indexes, i and $i_\perp$ stand for two orthogonal polarizations. E.g., one might choose the i's to represent horizontal-vertical, $\{H, V\}$, diagonal-antidiagonal, $\{45°, -45°\}$, or right-left handed circular, $\{R, L\}$, polarization analyzer settings. The zeroth Stokes operator is given by the total photon number operator $\hat{\Theta}_0 = \hat{N} = \hat{a}^{\dagger}{}_i\hat{a}_i + \hat{a}^{\dagger}{}_{i\perp}\hat{a}_{i_\perp}$[10].

If we are interested in the degree of polarisation of light we use $\left(\frac{\sum_i \langle\Theta_i\rangle^2}{\langle\Theta_0\rangle^2}\right)^{1/2}$. Obviously, this parameter is not a formal quantum observable (a self-adjoint linear operator). Neither is $\frac{\langle\Theta_i\rangle}{\langle\Theta_0\rangle}$. This is one of the reasons why attempts to build Bell inequalities using such parameters and their correlators for observation stations A and B in the form of $\frac{\langle\Theta_i^A\Theta_j^B\rangle}{\langle\Theta_0^A\Theta_0^B\rangle}$ fail and lead to misleading conclusions[11]. This is because such attempts involve additional assumptions, beyond the usual ones for Bell inequalities, which limit the range of local hidden variable theories for with such Bell inequalities must hold.

Bell inequalities for Stokes parameters can be formulated if one introduces normalized Stokes observables[12–14]:

$$\hat{S}_j = \hat{\Pi}\frac{\hat{n}_j - \hat{n}_{j_\perp}}{\hat{n}_j + \hat{n}_{j_\perp}}\hat{\Pi}, \tag{1}$$

where $\hat{\Pi} = \mathbb{I} - |\Omega\rangle\langle\Omega|$, and $|\Omega\rangle$ is the vacuum state (of the optical beam in question).

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It has been shown that such operators allow for the construction of stronger entanglement criteria, and they are a handy tool for formulation of Bell inequalities. One of their properties, crucial in this case, is the fact that these operators have a spectrum bounded by -1 and 1. That is, they have the basic property of observables which allows one to derive the CHSH-Bell inequalities. Thus, a derivation of a version of CHSH inequality applicable for such Stokes operators is essentially a replacement procedure. With the recent development of measurement techniques allowing photon number resolving detection[15,16] the discussion about normalized Stokes parameters stops to be only theoretical and its use in experiments is becoming feasible.

Note that what makes Pauli operators so straightforwardly applicable to Bell inequalities is their dichotomic nature. One of the attempts to construct field operators of a similar property was the formulation of pseudo-spin operators. For example, the z component of pseudo-spin is $(-1)^{\hat{n}}$, where $\hat{n}$ is the total photon number operator in the given optical mode[17,18]. The spectrum of pseudo-spin operators is the same as the spectrum of Pauli matrices, but their use introduces great difficulties from the experimental point of view. Even a loss of one photon (due to e.g. detector inefficiency) or a single dark count reverses the result of a measurement.

Here we analyze a simpler approach, which leads to proper Bell inequalities for polarization measurements of quantum optical fields. Our aim is to construct a family of operators that would have the usual spectrum for Bell experiments and would be robust with respect to experimental noise. We present polarization quantum field observables that have spectrum limited to ±1 and 0. Our initial ideas on such binning can be found in[19]. The approach to binning presented here is concurrent with the method used in[20] in the context of correlation in Bose-Einstein condensates. With the observables, we construct Bell inequalities. We test their resilience under losses and noise for 2×2 mode bright squeezed vacuum and bright GHZ radiation. The observables are realizable in the laboratory with standard measurement devices. They are described in the next section.

New operators: sign Stokes operators

It was shown that Bell inequalities constructed with normalized Stokes operators can be violated by macroscopic states of light such as 2×2 (bright) squeezed vacuum (BSV)[14] and its GHZ-like generalization (BGHZ)[21]. However, for a higher mean number of photons, the violation of Bell inequalities by these states is quickly damped. This results in lowering of the threshold values for pumping strength after which violation cannot be observed.

We address those problems by another normalization scheme, based on the so-called binning, which we call Sign approach normalization. To obtain new operators, we use the sign function and apply it to Stokes operators:

$$\hat{G}(s) = \text{sign}(\hat{n}_s - \hat{n}_{s_\perp}) = \text{sign}(\hat{\Theta}_s) = \text{sign}(\hat{U}_s(\hat{n}_H - \hat{n}_V)U_s^\dagger), \quad (2)$$

where s denotes the chosen setting related with the corresponding polarization basis with the eingenstates given by s and $s_\perp$. Subscripts H and V refer to horizontal and vertical polarizations, and the operator $\hat{U}_s$ is a unitary transformation that transforms the polarization modes H, V into another orthogonal pair of, in general, elliptic polarization modes $\{s, s_\perp\}$. From (2) we see that the eigenstates of $G(s)$ are $|j_s k_{s_\perp}\rangle = \frac{1}{\sqrt{j!k!}}\hat{a}_s^{\dagger j}\hat{a}_{s_\perp}^{\dagger k}|\Omega\rangle$, where $\hat{a}_s^\dagger$ and $\hat{a}_{s_\perp}^\dagger$ are creation operators related to the respective polarization modes of the given beam. The spectral form of (2) is given by:

$$\hat{G}(s) = \sum_{k>j}\Big(|k_s, j_{s_\perp}\rangle\langle k_s, j_{s_\perp}| - |j_s, k_{s_\perp}\rangle\langle j_s, k_{s_\perp}|\Big). \quad (3)$$

Formula (3) clearly shows that the new operators are well-defined Hermitian operators and that each $\hat{G}(i)$ has three eigenvalues ±1 and 0. Although formula (2) implies photon number operators, the basic idea of sign as well as standard and normalized Stokes operators is based on differences and sums of intensities. These in turn do not need to be modeled with photon counts. Note that formula (3) does not imply any particular model of intensity as long as the intensity increases with number of counts (even nonlinearly).

The action of the sign function on Stokes operators can be regarded as some form of the binning strategy used in the context of polarization measurements. Binning strategies are e.g. used in homodyne schemes for observing non-classicality[22–25].

We shall call the new operators sign Stokes operators. Following the usual approach, we shall define a triad of sign Stokes operators, related to the three maximally complementary settings of a polarization analyzer. For the usual triad of such settings, we denote by $\hat{G}_1$ the sign operator the eigenstates of which refer to $\{s = D, s_\perp = A\}$ polarization basis, and by $\hat{G}_2$ and $\hat{G}_3$ for respectively $\{R, L\}$ and $\{H, V\}$ bases. However, this notation is also extended to other triads of maximally complementary settings.

The sign operators share some properties of Stokes and normalized Stokes operators. Importantly, once one has a photon-number-resolving detection setup, the data collected in each run allows one to compute the obtained values of each of Stokes operators for the given basis i: standard, normalized, and sign ones, as they depend solely on the measured photon numbers n_i and $n_{i\perp}$. As we see, the new approach is in fact just a new form of data analysis that turns out to be simple and efficient. Further, in order to measure different sign operators $\hat{G}_{s'}$, that is, to move from s to s', it is enough to change the polarization analysis basis. Being useful from experimental point of view, unfortunately sign Stokes operators do not share all properties of quantum Stokes operators, what puts some limitations on their use in entanglement detection.

Stokes-like vector cannot be formed out of sign Stokes operators. Standard Stokes operators form a Stokes vector. We will discuss this property for pure states. However, it works also for mixed ones. We have $\langle\vec{\hat{\Theta}}\rangle_\psi = (\langle\hat{\Theta}_1\rangle_\psi, \langle\hat{\Theta}_2\rangle_\psi, \langle\hat{\Theta}_3\rangle_\psi)$ where $|\psi\rangle$ is an arbitrary state of the optical field. The Euclidean norm of this vector fulfills : $||\langle\vec{\hat{\Theta}}\rangle_\psi|| \leq \langle\hat{\Theta}_0\rangle_\psi$. We can construct an analogue vector for normalized Stokes operators and $||\langle\hat{\mathbf{S}}\rangle_\psi|| \leq \langle\hat{S}_0\rangle_\psi \leq 1$[13]. These norms remain invariant under any unitary transformation between two triads of mutually maximally complementary polarization analysers. This transformation can be put as $a_{3'} = U_{11}a_3 + U_{12}a_{3_\perp}$ and $a_{3'_\perp} = U_{21}a_3 + U_{22}a_{3_\perp}$, where U_{ij} are elements of a certain two-dimensional unitary matrix. Properly defined Stokes vector has its Euclidean norm invariant with respect to such mode transformations. As a transformation of this kind can also be expressed as a transformation of the state, one can introduce $|\psi'\rangle$, which is in the following relation with $|\psi\rangle$. If $|\psi\rangle = f(a_3^\dagger, a_{3_\perp}^\dagger)|\Omega\rangle$, then $f(a_{3'}^\dagger, a_{3'_\perp}^\dagger)|\Omega\rangle = |\psi'\rangle$, where $f(x, y)$ is a polynomial of both variables. We put this relation as $|\psi'\rangle = \hat{U}_{mode}^\dagger|\psi\rangle$, as it is obviously a specific unitary transformation of the state.

For such mode transformations we have $||\langle\hat{\vec{\Theta}}\rangle_\psi|| = ||\langle\hat{\vec{\Theta}}\rangle_{\psi'}||$ and $||\langle\hat{\vec{S}}\rangle_\psi|| = ||\langle\hat{\vec{S}}\rangle_{\psi'}||$. The norm of Stokes vectors, standard and normalized, is constant under any unitary transformation of the triads polarization analysis bases. These features of Stokes observables play a key role in the construction of entanglement indicators involving Stokes operators.

Such properties are not shared by sign operators. Let us construct $\langle\hat{\vec{G}}\rangle_\psi = (\langle\hat{G}_1\rangle_\psi, \langle\hat{G}_2\rangle_\psi, \langle\hat{G}_3\rangle_\psi)$. It can be shown that $||\langle\vec{G}\rangle_\psi|| \neq ||\langle\vec{G}\rangle_{\psi'}||$. It is enough to find one counterexample. Consider the state $|\psi\rangle = |3_H, 0_V\rangle$ i.e. the Fock state with 3 photons polarized horizontally. It can be easily checked that for this state $||\langle\vec{G}\rangle_\psi|| = 1$. Now let us apply a unitary transformation on optical modes of $|\psi\rangle$ such that the creation operators transform as follows: $\hat{a}_H^\dagger \rightarrow \hat{a}^\dagger(\alpha) = \cos\alpha\hat{a}_H^\dagger + \sin\alpha\hat{a}_V^\dagger$ and $\hat{a}_V^\dagger \rightarrow \hat{a}_\perp^\dagger(\alpha) = -\sin\alpha\hat{a}_H^\dagger + \cos\alpha\hat{a}_V^\dagger$. Let $\alpha = \pi/8$. One gets: $||\langle\vec{G}\rangle_{\psi'}|| \approx 1,5$. Thus, the norm is not an invariant of the unitary transformations, and additionally it is not bounded by 1. This fact prohibits one to use methods of construction of entanglement indicators presented in[13], which work via a simple replacement of Pauli operators in entanglement conditions for qubits, by Stokes operators, standard or normalized. Still, as we shall see, there is no obstacle to using this method in the case of construction of Bell inequalities.

Rotational *covariance* of polarization variables is not a necessary feature required to derive Bell inequalities (however, see[26] for the consequences of demanding exactly that). This allows one to construct CHSH and CH inequalities for fields with sign Stokes observables.

CHSH inequality. To derive Bell inequalities satisfied by any local realistic description, we start by defining local hidden values that predetermine the output of the measurement of sign Stokes operators (2). We denote the local hidden variables by λ. The functions $I^X(s, \lambda)$ and $I^X(s_\perp, \lambda)$ give the predetermined outcomes of the intensity measurements of polarizations $s, s_\perp$ in the local beam for the observer X. We define the local hidden values for sign operators as $G^X(s, \lambda) = \text{sign}(I^X(s, \lambda) - I^X(s_\perp, \lambda))$. These local hidden values are ± 1 and 0, thus one can use standard methods to derive CHSH inequality. The alternative settings will be denoted here by s, s' for the first observer and r, r' for the second observer. The resulting CHSH inequality reads:

$$|\langle G^1(s,\lambda)G^2(r,\lambda) + G^1(s,\lambda)G^2(r',\lambda) + G^1(s',\lambda)G^2(r,\lambda) - G^1(s',\lambda)G^2(r',\lambda)\rangle_{LHV}| \leq 2. \tag{4}$$

For further reference, we put it as $|CHSH_G| \leq 2$.

However, this inequality cannot be violated by states with a significant vacuum component, e.g. the (polarization) four-mode squeezed vacuum state, which will be our working example, see next sections. This situation is analogous to the case of normalized Stokes operators, see[14]. Following ideas of[14] we modify sign Stokes operators as follows:

$$\hat{G}^X(s) \rightarrow \hat{G}^{X-}(s) = \hat{G}^X(s) - \hat{\Pi}_{\Omega^X}, \tag{5}$$

where $\hat{\Pi}_{\Omega^X}$ is the projector on the subspace of the Fock space of states with no photons in the local beam. Such a projection allows for reduction of the impact of vacuum term, which often appears with the highest probability. Also local hidden values need to be modified:

- $G^{X-}(s, \lambda) = \text{sign}(I^X(s, \lambda) - I^X(s_\perp, \lambda))$ if $I^X(s, \lambda) + I^X(s_\perp, \lambda) \neq 0$
- $G^{X-}(s, \lambda) = -1$ if $I^X(s, \lambda) + I^X(s_\perp, \lambda) = 0$

As this modification does not change local hidden values $G^{X-}(s, \lambda) \in \{0, \pm 1\}$ we use the following CHSH inequality:

$$\begin{aligned} |CHSH_{G-}| = |\langle & G^{1-}(s,\lambda)G^{2-}(r,\lambda) + G^{1-}(s,\lambda)G^{2-}(r',\lambda) \\ & + G^{1-}(s',\lambda)G^{2-}(r,\lambda) - G^{1-}(s',\lambda)G^{2-}(r',\lambda)\rangle_{LHV}| \leq 2. \end{aligned} \tag{6}$$

Violation of Bell inequality for four mode squeezed vacuum—asymptotic behaviour. We are going to analyze how the use of sign Stokes operators in CHSH inequality helps to reveal the non-classicality of quantum states. Our working example is 2×2 mode squeezed vacuum state (BSV) which is the generalization of EPR singlet. It reads:

$$|\psi_-\rangle = \frac{1}{\cosh^2(\Gamma)} \sum_{n=0}^{\infty} \frac{\tanh^n(\Gamma)}{n!} (a_H^\dagger b_V^\dagger - a_V^\dagger b_H^\dagger)^n |\Omega\rangle = \frac{1}{\cosh^2(\Gamma)} \sum_{n=0}^{\infty} \sqrt{n+1} \tanh^n(\Gamma) |\psi^n\rangle, \tag{7}$$

where Γ is the amplification gain and

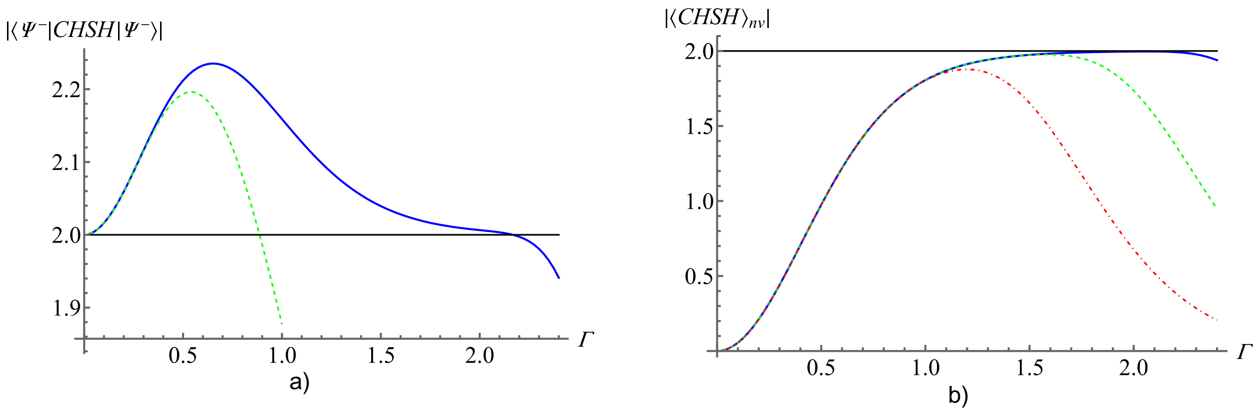

Figure 1. (**a**) The blue curve: the value of the $CHSH_{G-}$ expression based on sign operators, see (6), and the green dashed curve: $CHSH_{S-}$ based on normalized Stokes operators[14] in a function of amplification gain Γ of the *BSV* state. The numerical results were obtained with a cut-off of the expansion of the BSV state at the term $|\psi^{n=150}\rangle$. The maximal values of amplification gain (Γ_{tr}), such that for all $\Gamma < \Gamma_{tr}$ CHSH inequalities are violated, are $\Gamma_{tr} \approx 0.88$ for normalized Stokes operators[14] and $\Gamma_{tr} \approx 2.16$ for sign Stokes operators. Thus, with sign Stokes operators, the range of violation with respect to amplification gain is much larger than in the case of normalized Stokes operators. (**b**) The graphs show the non-vacuum term of $CHSH_{G-}$ as a function of amplification gain Γ for the BSV state, which was computed for cutoffs of 15, 47, 150 photons. This is done to illustrate that the descent of the curves for high Γ's is an artefact of the applied cutoff. The blue curve represents calculations with the cutoff at 150 photons,for the green dashed curve it is at 47 photons and for the red dot-dashed curve at 15 photons. The cutoff seems to be responsible for the decrease of the value in (**a**) for high Γ's.

$$|\psi^n\rangle = \frac{1}{\sqrt{n+1}} \sum_{m=0}^{n} (-1)^m |(n-m)_{H_1}, m_{V_1}, m_{H_2}, (n-m)_{V_2}\rangle. \quad (8)$$

Subscripts $H_{1_{(2)}}$ and $V_{1_{(2)}}$ specify the polarization of each mode and to which of the two optical beams it corresponds. We use the convention that $a_s^\dagger$ denotes the creation operator for the photon heading observer A, and $b_s^\dagger$ is the creation operator related to the observer B. The amplification gain determines the intensity of the pumping field and thus Γ sets the expectation value of the intensity of the BSV state.

Assume that both observers choose to measure only linear polarizations. thus, the angles by which the measurement polarization basis is rotated with respect to $\{H, V\}$ basis define the settings. With the notation used in "Stokes-like vector cannot be formed out of sign Stokes operators" section for unitary transformation between linear polarization modes we chose for the first observer $\alpha_s = 0$, $\alpha_{s'} = \pi/4$, and for the second one $\alpha_r = \pi/8$ and $\alpha_{r'} = -\pi/8$. It was shown that these settings are optimal in case of violation of CHSH inequality with normalized Stokes operators for BSV[14].

Figure 1 shows quantum predictions for $CHSH_{G-}$ (6) and the values of CHSH expression for normalized Stokes parameters for BSV taken from[14] as a function of the amplification gain Γ. Sign Stokes operators give $|\langle\psi_-|CHSH_{G-}|\psi_-\rangle| > 2$ for a wider range of an amplification gain that is up to $\Gamma_{tr} \approx 2.16$. For normalized Stokes operators, this maximal value of amplification gain is significantly lower, i.e. $\Gamma_{tr} \approx 0.8866$. Thus, with sign Stokes operators it is possible to reveal the non-classicality of BSV for a much higher value of amplification gain.

In Fig. 1 we can see that for $\Gamma \approx 2.1$ for sign Stokes operators $|CHSH_{G-}|$ drops down suspiciously suddenly. We presume that such behaviour might be a consequence of a cut-off. The expansion of $|\psi_-\rangle$ was cut off in the numerical calculations at $|\psi^{n=150}\rangle$. This still requires further investigation.

Because of the rotational invariance of $|\psi_-\rangle$, it is a "super-singlet", the expectation values of the correlators entering the Bell inequalities depend, if we measure linear polarizations on both sides, only on *relative angle* of the orientation of the polarization analyzers at the two spatially separated observation stations.

Note that standard, normalized, and sign Stokes operators are composed of functions of photon number operators, which do not change the number of photons. Thus, the expression $\langle\psi_-|CHSH_{G-}|\psi_-\rangle$ consists of two terms: *vacuum term*, that is CHSH inequality averaged over the vacuum component of BSV and *non-vacuum term*. The vacuum and non-vacuum terms in (6) for our settings are both negative. That is why we can consider the CHSH inequality in question as the sum of absolute values of these both terms. The vacuum term can be easily calculated:

$$|\langle\Omega|CHSH_{G-}|\Omega\rangle| = \frac{2}{\cosh^4\Gamma}. \quad (9)$$

The non-vacuum term $\langle CHSH_{G-}\rangle_{nv} = \langle\psi_-|CHSH_{G-}|\psi_-\rangle - \langle\Omega|CHSH_{G-}|\Omega\rangle$ results from the expectation values of $|\psi^n\rangle$. Note that as Γ increases, the role of non-vacuum terms in $\langle\psi_-|CHSH_{G-}|\psi_-\rangle$ increases too. For small Γ the contribution of vacuum term is dominant.

In Fig. 1 the value of the non-vacuum $|\langle CHSH_{G-}\rangle_{nv}|$ is presented. The calculation is performed for BSV state truncated to $n = 150$, blue curve, $n = 47$, green curve, and $n = 15$, red curve. These numbers increase approximately as a geometrical sequence by $\sqrt{10}$ what allows as to analyze the behaviour of $\langle CHSH_{G-}\rangle_{nv}$ within

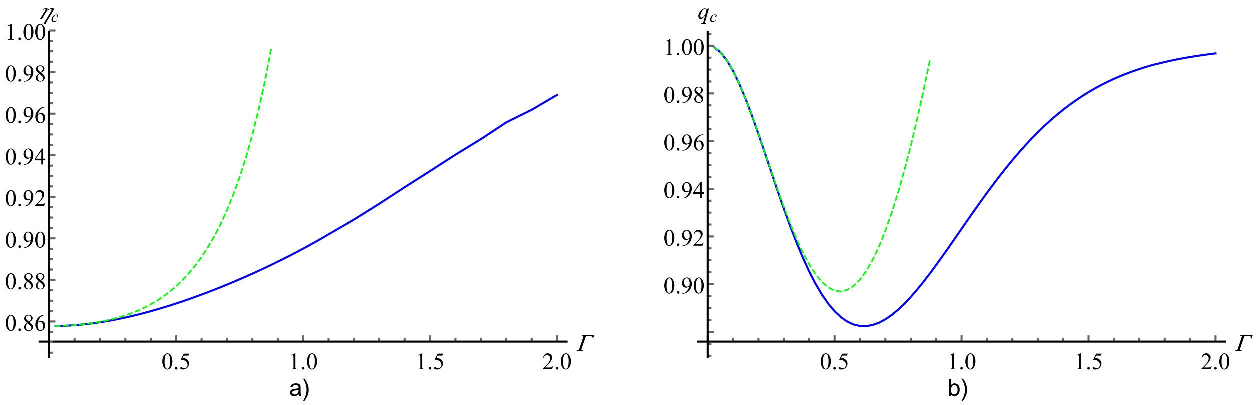

Figure 2. (**a**) Critical efficiency η_c versus Γ for the CHSH inequalities for the BSV state. A blue curve represents η_c for sign approach and a green dashed curve for normalized Stokes operators. (**b**) Critical value of q versus Γ for the BSV state. A blue curve represents q_c for sign approach and a green dashed curve for normalized stokes operators. Assuming that asymptotic behaviour of violation of CHSH inequality for sing parameters discussed in "Violation of Bell inequality for four mode squeezed vacuum—asymptotic behaviour" section is correct the q_c for the sign Stokes operators goes to 1 in the limit $\Gamma \to \infty$.

the whole order of magnitude. All curves asymptotically go to 2 (classical bound) up to some point for which they both start to decrease. Note that the curves for $n = 15$ and $n = 47$ start to decrease for smaller Γ than the curve for $n = 150$. It is highly probable that the decrease is conditioned by not including components with a high enough number of photons and the non-vacuum term $|\langle CHSH_{G-}\rangle_{nv}|$ goes asymptotically to 2 from the left. The vacuum term goes asymptotically to 0 from the right, see (9). Thus, our hypothesis is that CHSH inequality with sign Stokes operators is violated for BSV for any Γ. In Supplementary Discussion A we present a reasoning, based on a numerical calculation, supporting this conjecture.

CHSH inequality with losses. One of the crucial aspects of experimental realization of Bell experiments is detectors with high efficiency η. Here, we will analyze the critical value of efficiency η_c such that for $\eta < \eta_c$ one cannot observe a violation of (6). We model inefficient detectors in the standard way: a perfect detector ($\eta = 1$) with a beamspliter with transmissivity $\sqrt{\eta}$ in front of it. We denote by k the number of photons that reach the beamsplitter. Of these, only $\kappa \leq k$ counts are registered due to losses on the beamspliter. The probability of registration of κ photons is given by the binomial distribution:

$$p(\kappa|k) = \binom{k}{\kappa}\eta^{\kappa}(1-\eta)^{k-\kappa}. \tag{10}$$

In Fig. 2 we can see the minimal value of efficiency η_c for which the violation of CHSH inequality can be observed for normalized and sign Stokes operators in function of Γ. Note that for small Γ (up to $\Gamma \approx 0.3$) the curves for sign and normalized Stokes operators behave almost identically. However, as Γ increases, the value of η_c for sign Stokes operators grows slower than that for normalized ones. Such a change in rate of growth for a higher Γ should be expected because, for a high number of photons, loss of one photon matters less in the case of sign Stokes operators.

CHSH inequality with noise. In a realistic scenario of a Bell experiment apart from photon losses one shall consider also noise. Our noise is modeled in the similar way as "white noise" for qubits. Let us introduce four squeezed vacuum states which are related with the Bell state basis for two qubits[27]:

$$|\Phi^{\pm}\rangle = \frac{1}{\cosh^2(\Gamma)}\sum_{n=0}^{\infty}\frac{\tanh^n(\Gamma)}{n!}(a_H^{\dagger}b_H^{\dagger} \pm a_V^{\dagger}b_V^{\dagger})^n|\Omega\rangle, \tag{11}$$

and

$$|\Psi^{\pm}\rangle = \frac{1}{\cosh^2(\Gamma)}\sum_{n=0}^{\infty}\frac{\tanh^n(\Gamma)}{n!}(a_H^{\dagger}b_V^{\dagger} \pm a_V^{\dagger}b_H^{\dagger})^n|\Omega\rangle. \tag{12}$$

Our noise model can be defined as follows:

$$\rho_{noise} = \frac{1}{4}(|\phi^+\rangle\langle\phi^+| + |\phi^-\rangle\langle\phi^-| + |\psi^+\rangle\langle\psi^+| + |\psi^-\rangle\langle\psi^-|). \tag{13}$$

Note that ρ_{noise} is uncorrelated. Let q be the visibility. The noisy state reads:

$$\rho' = q|BSV\rangle\langle BSV| + (1-q)\rho_{noise}, \tag{14}$$

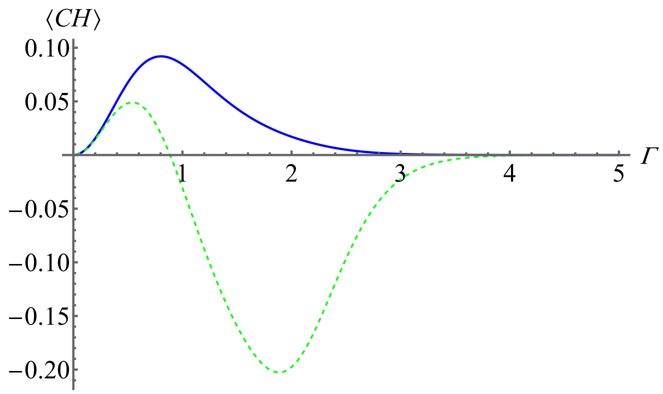

Figure 3. Quantum predictions for expectation value of CH expression for the 'sign' approach (blue curve) and rate approach[14] (green dashed curve) as a function of the amplification gain Γ for BSV state. The numerical results were obtained with a cut-off of the expansion of the BSV state at the term $|\psi^{n=50}\rangle$. The upper bound of CH inequality for the 'sign' approach is violated in the whole range of Γ covered in the figure, while the violation of the inequality in the case of the normalized Stokes operators is quickly damped and after that CH expression goes asymptotically from bellow to the classical bound.

The value $1-q$ determines the probability of registering noise. Figure 2 shows the minimal value of visibility q_c that ensures the violation of CHSH inequality for normalized and Stokes operators. We see that sign Stokes operators have a similar advantage over normalized Stokes operators as in the case of losses, i.e. for small Γ normalized and sign Stokes operators are similarly resistant to noise. As Γ increases sign Stokes operators result to be significantly more efficient, Moreover from the results shown on Fig. 2 and the reasoning presented in "Violation of Bell inequality for four mode squeezed vacuum—asymptotic behaviour" section we can conclude that $q_c \to 1$ when $\Gamma \to \infty$.

CH inequality. Going along with the idea of sign operators and rate approach to CH inequality[14] we can construct a new CH inequality for quantum optical fields. Let us move directly to the quantum scenario and start with the CH operator (CH_R) for intensity rates. In[14] the rates are defined by $\hat{R}_+(s) = \hat{\Pi}\hat{n}_s/(\hat{n}_s + n_{s_\perp})\hat{\Pi}$. Note that such an operator is simply the first term of normalized Stokes operator (1). Its eigenvalues are rational numbers in (1/2, 1] for photon number states $|n_s, m_{s_\perp}\rangle$ where $n > m$ and in [0, 1/2) for states where $n < m$. If $m = n$ the eigenvalue of the rates is 1/2. Combining the idea CH inequality for rates and the concept sign Stokes operators we construct operators for CH inequality based binning. We seek for operators of eigenvalues with the following properties: we have 1 when $m > n$ and 0 if $n \leq m$. Such a dichotomic observable is simply a projector onto subspace $n > m$:

$$\hat{P}(s) = \sum_{n>m} |n_s, m_{s_\perp}\rangle\langle n_s, m_{s_\perp}|. \tag{15}$$

The expectation value of $\hat{P}^X(s)$ is equal to the probability that the observer X will see $n > m$. We shall denote by $\langle \hat{P}^X(j)\hat{P}^Y(k)\rangle$ the quantum joint probability of obtaining the same result $n > m$ by observers X and Y for their respective polarization basis j and k. Had these probabilities in the experiment been classical, and if the assumptions of local realism hold Clauser–Horne inequality tailored for the quantum scenario is given by:

$$-1 \leq \langle CH_P\rangle = \left\langle \hat{P}^1_+(\theta)\hat{P}^2_+(\phi) + \hat{P}^1_+(\theta)\hat{P}^2_+(\phi') + \hat{P}^1_+(\theta')\hat{P}^2_+(\phi) - \hat{P}^1_+(\theta')\hat{P}^2_+(\phi') - \hat{P}^1_+(\theta) - \hat{P}^1_+(\phi) \right\rangle \leq 0. \tag{16}$$

Figure 3 shows the expectation value of the CH expression (16) and its rate counterpart for the same settings as in the case of CHSH inequality. The 'sign' approach gives violation of upper bound of CH expression for all Γ while the rate approach gives a violation only for $\Gamma < 0.8866$ which is the same case as for CHSH. Note that this CH inequality is not equivalent to CHSH inequality (6) (see Supplementary Discussion A)

Violation of Bell inequalities with sign approach for Bright GHZ state

As another example, let us consider a Bright GHZ state which is a generalization of the two beam squeezed vacuum considered above, to three beam emissions.

Such a process for years was thought to be infeasible, but current experimental progress allows one to think of such a possibility. The usual parametric approximation of the theoretical description of generation process of such states, which describes the pumping field as classical, does not work because of the divergence of perturbation series. Still, with an employment of a version of Padè approximation one can find an approximate parametric description, with convergent perturbation series, see[21]. The approximation gives a state of the following form:

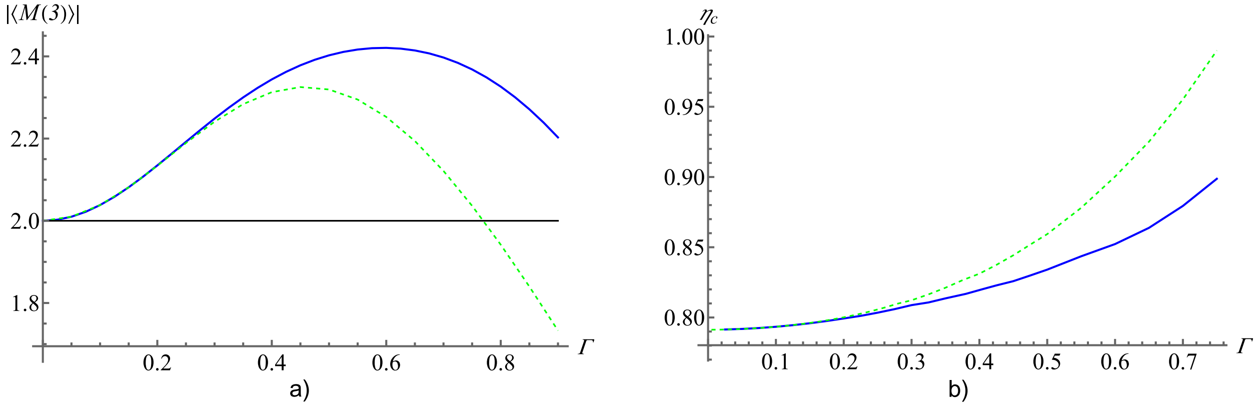

Figure 4. (**a**) Quantum values of $|M(3)_{G-}|$ expression (blue curve) and $|M(3)_{S-}|$ (green dashed curve) as a function of the amplification gain Γ for BGHZ state. (**b**) Critical efficiency η_c versus Γ for Mermin inequalities for the BGHZ state. The blue curve represents η_c for the sign approach and a green dashed curve for normalized Stokes operators.

$$|BGHZ\rangle = \sum_{k=0}^{\infty}\sum_{m=0}^{k} C_{k-m}(\Gamma)C_m(\Gamma)(\hat{a}_i^\dagger \hat{b}_i^\dagger \hat{c}_i^\dagger)^{k-m}(\hat{a}_{i_\perp}^\dagger \hat{b}_{i_\perp}^\dagger \hat{c}_{i_\perp}^\dagger)^m|\Omega\rangle. \tag{17}$$

The method of obtaining the coefficients $C_m(\Gamma)$ can be found in[21], and we base our numerical computations on the results established in this reference. The symbols $\hat{a}_p^\dagger$, $\hat{b}_p^\dagger$ and $\hat{c}_p^\dagger$ stand for creation operators in two orthogonal polarization modes $p = i, i_\perp$, of a beam which goes to respectively observers A, B and C. For simplicity, we assumed the polarization modes to be H, V, that is, $i = 3$.

Mermin-like inequality. Let us consider Mermin-like inequality for quantum optical fields[21]:

$$|M(3)_S| = |\langle S_1^1(\lambda)S_1^2(\lambda)S_1^3(\lambda) - S_1^1(\lambda)S_2^2(\lambda)S_2^3(\lambda) - S_2^1(\lambda)S_1^2(\lambda)S_2^3(\lambda) - S_2^1(\lambda)S_2^2(\lambda)S_1^3(\lambda)\rangle_{LHV}| \le 2, \tag{18}$$

where $S_i^X(\lambda)$ are local hidden values corresponding to normalized Stokes operators with polarization bases: $\{45°, -45°\}$, $\{R, L\}$, for $i = 1, 2$ respectively. The observers are now marked by $X = 1, 2, 3$. The inequality (18) generalizes Mermin inequality for three qubits[28] for three photon beams with two polarisation modes each from a parametric source, for details see:[21]. Of course, in general the settings 1, 2 could be different.

The derivation of this inequality requires only that local hidden values are bounded by ± 1. Because local hidden values for sign Stokes operators fulfil this requirement, we can replace $S_i^X(\lambda)$ by $G_i^X(\lambda)$ and obtain a new inequality

$$|M(3)_G| = |\langle G_1^1(\lambda)G_1^2(\lambda)G_1^3(\lambda) - G_1^1(\lambda)G_2^2(\lambda)G_2^3(\lambda) - G_2^1(\lambda)G_1^2(\lambda)G_2^3(\lambda) - G_2^1(\lambda)G_2^2(\lambda)G_1^3(\lambda)\rangle_{LHV}| \le 2. \tag{19}$$

However, this inequality is not violated by the BGHZ state. We have to again modify sign Stokes operators (as well as normalized Stokes operators):

$$\hat{G}_i^X \to \hat{G}_i^{X-} = \hat{G}_i^X - \hat{\Pi}_{\Omega^X}. \tag{20}$$

One can easily write modified local hidden values for such operators as in "CHSH inequality" section and obtain inequality:

$$\begin{aligned} |M(3)_{G-}| = |\langle & G_1^{1-}(\lambda)G_1^{2-}(\lambda)G_1^{3-}(\lambda) - G_1^{1-}(\lambda)G_2^{2-}(\lambda)G_2^{3-}(\lambda) \\ & - G_2^{1-}(\lambda)G_1^{2-}(\lambda)G_2^{3-}(\lambda) - G_2^{1-}(\lambda)G_2^{2-}(\lambda)G_1^{3-}(\lambda)\rangle_{LHV}| \le 2. \end{aligned} \tag{21}$$

Figure 4 presents quantum values of $|\langle BGHZ|\hat{M}(3)_{G-}|BGHZ\rangle|$ and of analogous expression, $|\langle BGHZ|\hat{M}(3)_{S-}|BGHZ\rangle|$, for a Mermin inequality for modified normalized Stokes operators, $\hat{S}_i^{X-} = \hat{S}_i^X - \hat{\Pi}_{\Omega^X}$, which is of the form (18) with $\hat{S}_i^{X-}$ replacing $\hat{S}_i^X$. All that is with respect to the amplification gain Γ. The range of Γ for which the inequality is violated by BGHZ state in the case of sign Stokes operators exceeds the range of applicability of the method used to approximate the probability amplitudes for BGHZ state. We also stress that this result is more robust than in the case of normalized Stokes operators. The graphs in Fig. 4 are discontinued at $\Gamma = 0.9$ because for higher values the approximation of ref.[21] breaks down.

Mermin-like inequality with losses. We use the model of losses due to inefficient detectors as in "CHSH inequality with losses" section for the inequality (21). In Fig. 4 critical values of efficiency of detectors η_c, for sign and normalized Stokes operators, are compared. We can see that for small Γ inequalities exhibit similar resistance to losses. However, with increasing Γ difference between the performance of sign and normalized Stokes observables increases in favour of the former ones.

Conclusions and some open questions

We have proposed, based on a version of the binning approach[19,20], new Stokes-like polarization observables for quantum optical fields which have a clear operational meaning. In presented examples, the sign Stokes observables allow observation of Bell non-classicality of squeezed-vacuum-type states for pumping powers, for which normalized Stokes observables fail to do so. Sign Stokes operators are easier in experimental realization than normalized ones. Also, they are more resistant to imperfect detection and presence of a noise. One could be tempted to use sign Stokes observables to derive entanglement indicators not based on Bell inequalities. However, such Stokes observables do not possess properties which are commonly used in derivations of bounds for separable states. Simply a triad of them does not form a Stokes vector with proper covariance properties. Thus, this requires a different approach. Similar questions arise when one thinks of a steering condition involving sign Stokes observables.

Another question would be if there is a type of state for which normalized Stokes operators allow for violating of some Bell inequality and for which this is impossible using sign Stokes operators.

The presented results give a possible way to search for violations of local realism in situations with undefined particle numbers, which are so common in especially quantum optics. The associated Bell inequalities are correctly defined. That is, the sole assumption is local realism (and tacitly freedom of the choice of the random settings for all observers involved). No additional "reasonable" assumptions are used. As, according to our numerical estimates, one can conjecture that the associated inequalities are violated for an arbitrary Γ, they may serve as tool to reveal Bell non-classicality of bright quantum optical states, see[29]. This indicates that such states may find an application in, e.g. quantum communication, provided one finds new suitable Bell inequalities which would lead to more robust violations of local realism.

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Author contributions

All authors contributed equally to this work.

Competing interests

The authors declare no competing interests.

Additional information

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Simplified Quantum Optical Stokes observables and Bell's Theorem - Supplementary Discussion

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1 Supplementary Discussion A: Asymptotic violation of CHSH inequality

Here we present the numerical argumentation for our hypothesis that CHSH inequality (6) with sign Stokes operators is violated for BSV for any Γ.

Let us start with the analysis of quantum predictions for expectation values of (6) for states $|\psi^n\rangle$ i.e. $|\langle CHSH_{G-}\rangle_{\psi^n}|$, for $n \neq 0$, and compare them with analogue expression for normalized Stokes operators.

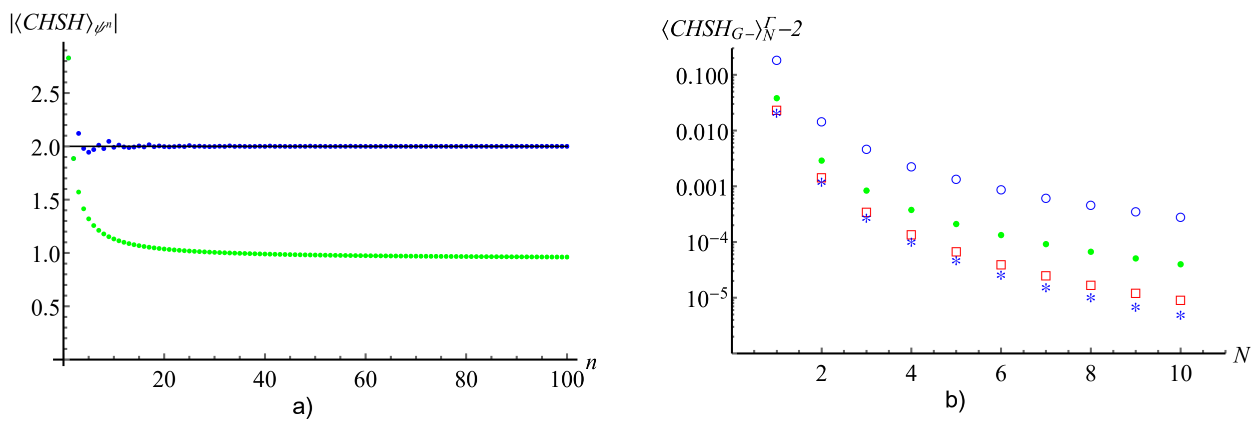

Figure 1. a) $\langle CHSH_{G-}\rangle_{\psi^n}$ for sign Stokes operators (blue points) and analogue for normalized Stokes operators $\langle CHSH_{S-}\rangle_{\psi^n}$ (green points) operators for $|\psi^n_-\rangle$ as a function of n. The points: $n=1$ and $n=2$ of both approaches coincide. For normalized Stokes operators only singlet state contribute to the violation and all points converge to 1 which is the bound for separable states. In the case of sign Stokes operators all points are concentrated around the classical bound for CHSH inequality. b) $\langle CHSH_{G-}\rangle_N^{(\Gamma)}$ versus N. $\Gamma=1$ circles, $\Gamma=2$ dots, $\Gamma=3$ squares, $\Gamma\to\infty$ stars. For any Γ values of $\langle CHSH_{G-}\rangle_N^{(\Gamma)}$ go to 2 with growing N. The case of $\Gamma\to\infty$ bounds $\langle CHSH_{G-}\rangle_N^{(\Gamma)}$ from bellow.

FIG.1 shows results for $n=1,\ldots,100$ for sign Stokes operators and normalized Stokes operators. For normalized Stokes operators only for $n=1$ we get $|\langle CHSH_{S-}\rangle_{\psi^n}|\geq 2$. For sign operators, the values of $|\langle CHSH_{G-}\rangle_{\psi^n}|$ concentrate around 2 with growing n. More detailed analysis (see FIG. 2) reveals two patterns: an oscillating one for odd n's and a pattern converging to 2 from below for even n's. The period of odd n's is equal to $T=8$ in the sense that points $n=2k+1$ and $n=2k+1+T$ where $k\in\mathbb{N}$ corresponds to e.g. two adjacent maximums in the pattern. The even pattern also has an internal structure repeatable with $T=8$.

The periodicity of the pattern values being above and below 2 provides us the natural grouping of $|\langle CHSH_{G-}\rangle_{\psi^n}|$. Let us examine a weighted average $\langle CHSH_{G-}\rangle_N^{(\Gamma)}$ of $|\langle CHSH_{G-}\rangle_{\psi^n}|$ for a given Γ over N-th period for $\Gamma>2$:

$$\langle CHSH_{G-}\rangle_N^{(\Gamma)} = \frac{\sum_{n=1+T(N-1)}^{T+T(N-1)} |\langle CHSH_{G-}\rangle_{\psi^n}|\,|\langle\psi^n_-|\psi_-\rangle|^2}{\sum_{n=1+T(N-1)}^{T+T(N-1)} |\langle\psi^n_-|\psi_-\rangle|^2}, \tag{A1}$$

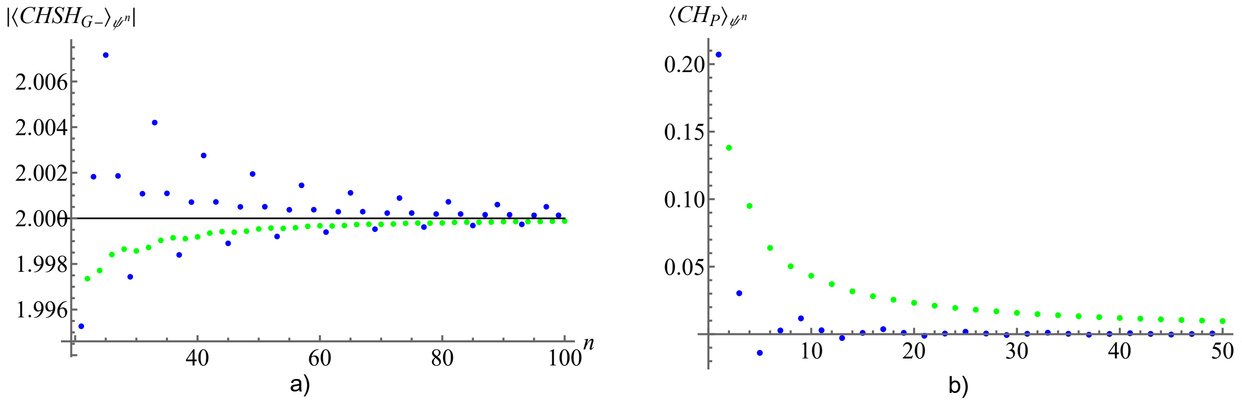

Figure 2. a) $\langle CHSH_{G-}\rangle_{\psi^n}$ versus n. Blue darker dots depict odd n and green dots stand for even n. We can observe two patterns occurring. The first pattern for odd n' oscillates around the bound with decreasing amplitude and period $T=8$. The second pattern for even n' converges to 2 from below with growing n. This pattern also has an internal structure which is repeatable with $T=8$ (increase, decrease, increase, increase). Note that only $\left|\psi_-^n\right\rangle$ with odd n violate $CHSH$ inequality for sign Stokes operators. However, not all $\left|\psi_-^n\right\rangle$ for odd n exhibit non-classical correlations. Still, for every n in the odd pattern for which there is no violation (6) we have 3 different odd n' for which violation occurs. b) Quantum predictions of $\langle CH_P\rangle$ for $\left|\psi_-^n\right\rangle$ versus n. Blue darker dots depict odd n and green dots stand for even n. In this case, there are also two patterns. The oscillating odd pattern with the same properties and the convergent even pattern. However, in this case, the even pattern goes to bound from above, and clearly have a higher impact on violation of (16) by the BSV state. This shows that CH inequality (16) is not equivalent to CHSH inequality (6).

where $|\left\langle \psi_-^n \middle| \psi_- \right\rangle|^2 = (n+1)\frac{\tanh^{2n}\Gamma}{\cosh^4\Gamma}$. Fig. 1 shows values of $\langle CHSH_{G-}\rangle_N^{(\Gamma)} - 2$ for $\Gamma = 1,2,3$ and $\Gamma \to \infty$.

We observe that $\langle CHSH_{G-}\rangle_N^{(\Gamma)}$ is a decreasing function of Γ. All calculated values of $\langle CHSH_{G-}\rangle_N^{(\Gamma)}$ exceed 2 and violate the inequality (6). Also $\langle CHSH_{G-}\rangle_N^{(\Gamma)}$ for any given Γ converges to 2 with growing N. Moreover the curve corresponding to $\Gamma \to \infty$ is the most relevant for our analysis because it bounds the $\langle CHSH_{G-}\rangle_N^{(\Gamma)}$ from bellow.

We recall that the quantum prediction for the expectation value of the CHSH inequality (6) consists of two terms: the vacuum term and the non-vacuum term:

$$|\langle \psi_- | CHSH_{G-} | \psi_- \rangle| = |\langle \Omega | CHSH_{G-} | \Omega \rangle| + |\langle CHSH_{G-}\rangle_{nv}| = \frac{2}{\cosh^4\Gamma} + |\langle CHSH_{G-}\rangle_{nv}|. \tag{A2}$$

The non-vacuum term $\langle CHSH_{G-}\rangle_{nv}$ can be written as the weighted average of $\langle CHSH_{G-}\rangle_N^{(\Gamma)}$:

$$|\langle CHSH_{G-}\rangle_{nv}| = \sum_{N=1}^{\infty} \langle CHSH_{G-}\rangle_N^{(\Gamma)} \sum_{n=1+T(N-1)}^{T+T(N-1)} |\left\langle \psi_-^n \middle| \psi_- \right\rangle|^2. \tag{A3}$$

Assuming that there is no change in the pattern of $\langle CHSH\rangle_{\psi^n}$ as n increases (see the discussion below) we can bound from below the value of $|\langle CHSH_{G-}\rangle_{nv}|$ by replacing $\langle CHSH_{G-}\rangle_N^{(\Gamma)}$ with 2:

$$|\langle CHSH_{G-}\rangle_{nv}| \geq \sum_{n=1}^{\infty} 2(n+1)\frac{\tanh^{2n}\Gamma}{\cosh^4\Gamma} = 2(\tanh^2\Gamma + \mathrm{sech}^2\Gamma \tanh^2\Gamma). \tag{A4}$$

Equality due to our assumptions should be only reached in the limit of $\Gamma \to \infty$. This is because in the regime of high values of Γ only terms with high n are significant and $\langle CHSH_{G-}\rangle_N^{(\Gamma)}$ from the assumption reach 2 only when $N \to \infty$. Expression (A4) as expected has an asymptotic value 2. If we add the vacuum term to the RHS of (A4) we obtain constant function equal to 2. Thus, the above reasoning supports the conjecture that for any Γ:

$$|\langle \psi_- | CHSH_{G-} | \psi_- \rangle| \geq 2. \tag{A5}$$

Finally, let us argue why for higher n's the same pattern is expected. Note that $\left|\psi_-^n\right\rangle$ can be written in the following form:

$$\left|\psi_-^n\right\rangle = \frac{1}{n!\sqrt{n+1}}(\hat{a}_H^\dagger \hat{b}_V^\dagger - \hat{a}_V^\dagger \hat{b}_H^\dagger)^n \left|\Omega\right\rangle . \tag{A6}$$

Given some point in the pattern $\langle CHSH_{G-}\rangle_{\psi^n}$ to obtain the next corresponding point in the pattern we only have to apply operator $(\hat{a}_H^\dagger \hat{b}_V^\dagger - \hat{a}_V^\dagger \hat{b}_H^\dagger)^T$ to the state $\left|\psi_-^n\right\rangle$ and normalize it by the factor $\frac{n!\sqrt{n+1}}{(n+T)!\sqrt{n+T+1}}$. To obtain the next k-th corresponding point we have to apply this operator k times. Thus, applying such operator has to preserve some internal symmetries. There is no reason for existence of k such that it suddenly stops to preserve those symmetries. Therefore, the pattern should be continued for any period N.

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Bosonic fields in states with undefined particle numbers possess detectable non-contextuality features, plus more

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Abstract

The paradoxical features of quantum theory are usually formulated for fixed number of particles. While one can now find a formulation of Bell's theorem for quantum fields, a Kochen–Specker-type reasoning is usually formulated for just one particle, or like in the case of Peres–Mermin square for two. Is it possible to formulate a contextuality proof for situation in which the numbers of particles are fundamentally undefined? We introduce a representation of the $\mathfrak{su}(2)$ algebra in terms of boson number states in two modes that allows us to assess nonclassicality of states of bosonic fields. This representation allows to show contextuality, and is efficient to reveal violation of local realism, and to formulate entanglement indicators. A form of an non-contextuality inequality is derived, giving a bosonic Peres–Mermin square. The entanglement indicators are built with Pauli-like field observables. The non-clasicality indicators are effective. This is shown for the 2×2 bright squeezed vacuum state, and a recently discussed bright-GHZ state resulting from multiple three photon emissions in a parametric process.

1. Introduction

Quantum phenomena without any classical analogue are the fuel of many protocols of interest in quantum technologies, constituting the main resources for their different applications. To name a few, contextuality has been addressed as the key ingredient providing the speed-up in quantum computation over the classical one [1], the violation of a Bell inequality enables one to implement secure cryptographic schemes [2] and entangled probes allow one to achieve better precision in metrological tasks [3].

In parallel, research on the quantum properties of bosonic fields, notably first of all quantum light, has constituted one of the pillars in the development of quantum technologies, and it is still of paramount importance. Nonclassicality of a state of a quantum field can be revealed in many ways, ranging from looking at the negativity or singularity of a certain quasi-distribution function [4], to criteria to establish the nonseparability of a multimode field [5]. Following the approaches borrowed from finite-dimensional systems, another strategy to show whether a field admits a classical description or not is to introduce a set of inequalities that are fulfilled by measurement probabilities which are possible to model by a classical local-realistic theory, but are violated when taking into account the quantum mechanical predictions.

If the local hidden variable theory imposes some constraints on the structure of the joint probabilities or on the statistical correlations of measurements on multipartite systems, then these constraints can usually be put in a form of linear Bell inequalities. While if we consider hidden variable theories in which predetermined measurement values of any (degenerate) observable do not depend on the context in which the observable is measured, then the constraints are of Kochen–Specker type. A context is defined by a non-degenerate observable, which commutes with the observable in question, see e.g. [6].

Here, we focus on the quantification of different forms of nonclassicality for optical fields introducing a suitable set of operators defined in terms of the number states of two modes of the field. Their mathematical expressions are handy and allow us to map some results derived for qubit-systems to optical states. We remark here that, despite our efforts, we still do not have a clear picture of how such measurements can be implemented in an experimental scenario. This poses an interesting experimental challenge.

2. Pauli-like operators for bosonic fields

Let us introduce a set of Hermitian operators for optical fields which generalize the Pauli matrices in a Fock space describing two distinguishable modes of a bosonic field:

$$\begin{aligned}\hat{G}_0 &= \mathbb{1} - \sum_n |n,n\rangle\langle n,n|,\\ \hat{G}_1 &= \sum_{n\neq m} |n,m\rangle\langle m,n|,\\ \hat{G}_2 &= -\mathrm{i}\ \mathrm{sign}(\hat{a}^\dagger\hat{a} - \hat{b}^\dagger\hat{b})\sum_{n\neq m}|n,m\rangle\langle m,n|,\\ \hat{G}_3 &= \mathrm{sign}(\hat{a}^\dagger\hat{a} - \hat{b}^\dagger\hat{b}),\end{aligned} \tag{1}$$

where $\hat{a}^\dagger, \hat{b}^\dagger$ are creation operators of two orthogonal bosonic modes, $\mathbb{1}$ is the two mode identity and $|n,m\rangle = \frac{1}{\sqrt{n!m!}}a^{\dagger n}b^{\dagger m}|\Omega\rangle$, with $|\Omega\rangle$ being the vacuum. Function sign(x) gives ± 1 for $x \in \mathbb{R}^\pm$ and 0 for $x = 0$. The operator $\hat{G}_3$ coincides with one of sign Stokes operators introduced in [7]. The operators $\hat{G}_i$ can also be written in more compact form:

$$\hat{G}_i = \begin{pmatrix}\hat{S}_R^\dagger & \hat{P}_R^\dagger\end{pmatrix}\sigma_i\begin{pmatrix}\hat{S}_R\\ \hat{P}_R\end{pmatrix} = \vec{V}^\dagger\sigma_i\vec{V}, \tag{2}$$

where σ_i is the ith Pauli matrix, $\vec{V}^\dagger = \begin{pmatrix}\hat{S}_R^\dagger & \hat{P}_R^\dagger\end{pmatrix}$ and

$$\hat{P}_R = \sum_{m>n}|n,m\rangle\langle n,m|, \tag{3}$$

$$\hat{S}_R = \sum_{m>n}|n,m\rangle\langle m,n|. \tag{4}$$

These operators fulfill the same commutation relation as Pauli matrices:

$$[\hat{G}_i, \hat{G}_j] = 2\mathrm{i}\epsilon_{ijk}\hat{G}_k, \tag{5}$$

where $i, j, k = 1, 2, 3$. They also fulfill the anticommutation relation:

$$\{\hat{G}_i, \hat{G}_j\} = 2\delta_{ij}\hat{G}_0, \tag{6}$$

and from that follows (for details, see appendix A):

$$\hat{G}_i\hat{G}_j = \delta_{ij}\hat{G}_0 + \mathrm{i}\epsilon_{ijk}\hat{G}_k. \tag{7}$$

The $\hat{G}_0$ operator plays an analogous role of the identity, i.e. $\hat{\sigma}_0 = \mathbb{1}$, and obviously it commutes with all the other G_i operators. Since these operators satisfy the commutation relation in (5), they are a representation of the two-boson $\mathfrak{su}(2)$ algebra. Such a representation has advantages over the standard two mode representation of $\mathfrak{su}(2)$ [8] given by:

$$\hat{S}_i = \frac{1}{2}A^\dagger\sigma_i A, \tag{8}$$

where $A^\dagger = (\hat{a}^\dagger, \hat{b}^\dagger)$. The new set of operators defined in the equations in (1) fulfills the anticommutation relation (6), in contrast to the Stokes operators in equation (8). The anticommutation property turns to be crucial in a generalization of the Peres–Mermin square for bosonic fields, because it will let us recover the algebra of the tensor product of Pauli operators acting on two qubits. Moreover, the $\hat{G}_i$ operators are bounded (see appendix B) contrary to those previously introduced in (8). We remark that the new operators *under unitary transformation of the modes* do not form an equivalent $\mathfrak{su}(2)$ representation. In fact, given two sets of new operators, G_i and G_i', for different modes basis namely $\hat{a}, \hat{b}$ and $\hat{a}', \hat{b}'$, they are not linked through unitary transformation of the modes (see appendix C) as it is for the Stokes operator defined in (8).

3. Contextuality for quantum optical fields

The Kochen–Specker theorem [9] asserts that quantum mechanics is not compatible with any local hidden variable noncontextual theory. Here, noncontextuality means that the value for an observable predicted by such a theory is independent of the experimental context, namely the set of other co-measurable observables are simultaneously measured. In classical physics, the measurement outcomes of several observables do not depend on the order in which such quantities are measured. At the same time, quantum mechanics forbids existence of joint probability distributions for non-compatible observables. Noncontextual description of quantum measurements has been experimentally falsified for systems with a definite number of particles [10, 11]. However, few attempts have been proposed till now to quantify and measure it for systems allowing states with an undefined number of particles, such as quantum optical fields [12, 13]. Finding such examples is not an academic question, as one can imagine that in future there might be quantum informational processes based on such systems and such states.

3.1. Peres–Mermin square for optical observables

We introduce a version of the Peres–Mermin square [14, 15] for the 2×2 mode states of quantum optical fields, given that the operators $\hat{G}_i$ fulfill (7) as Pauli matrices do. Following the convention already introduced in [12], we denote by $\hat{A}_{pq}$ observables such that if two of those observables share a common index, they commute, i.e., the order in which they are measured does not have an impact on the outcome. We chose nine of such observables by mapping the Peres–Mermin square in the following way $\hat{\sigma}_i^1 \otimes \hat{\sigma}_j^2 \rightarrow \hat{G}_i^1 \hat{G}_j^2$, where superscripts denote the measuring parties. The Peres–Mermin square for the set of observables of the quantum optical fields reads:

$\hat{A}_{ij}$	$j = 1$	$j = 2$	$j = 3$
$i = 1$	$\hat{G}_3^1\hat{G}_0^2$	$\hat{G}_0^1\hat{G}_3^2$	$\hat{G}_3^1\hat{G}_3^2$
$i = 2$	$\hat{G}_0^1\hat{G}_1^2$	$\hat{G}_1^1\hat{G}_0^2$	$\hat{G}_1^1\hat{G}_1^2$
$i = 3$	$\hat{G}_3^1\hat{G}_1^2$	$\hat{G}_1^1\hat{G}_3^2$	$\hat{G}_2^1\hat{G}_2^2$

Following the method proposed in [16] to test whether quantum mechanics violates the bound imposed by a noncontextual hidden variable (NCHV) theory, we consider the following operator:

$$\hat{O} = \hat{A}_{11}\hat{A}_{12}\hat{A}_{13} + \hat{A}_{21}\hat{A}_{22}\hat{A}_{23} + \hat{A}_{31}\hat{A}_{32}\hat{A}_{33} + \hat{A}_{11}\hat{A}_{21}\hat{A}_{31} + \hat{A}_{12}\hat{A}_{22}\hat{A}_{32} - \hat{A}_{13}\hat{A}_{23}\hat{A}_{33}, \tag{9}$$

where, in each term, one index is shared among the three operators $\hat{A}_{pq}$. We make here an observation: the observables we have introduced are not dichotomic, whereas they have spectrum $\{-1, 0, 1\}$. This is in contrast to the observable used in the original construction of the Peres–Mermin square, namely the spin$-\frac{1}{2}$ observables. However, the maximal average value of the expression (9) in a NCHV model computed via the method given in [16] yields the same value 4, both for dichotomic observables and for our generalized Pauli-observable for two radiation modes. Thus, we obtain the inequality:

$$\langle A_{11}A_{12}A_{13} + A_{21}A_{22}A_{23} + A_{31}A_{32}A_{33} + A_{11}A_{21}A_{31} + A_{12}A_{22}A_{32} - A_{13}A_{23}A_{33}\rangle_{\text{NCHV}} \leqslant 4. \tag{10}$$

For the quantum case we observe that the first five terms of (9) have the same form $\hat{G}_0^1\hat{G}_0^2$ and the last term is equal to $-\hat{G}_0^1\hat{G}_0^2$. Thus, as expected $\mathbb{1} \rightarrow \hat{G}_0$. The operator $\hat{G}_0^1\hat{G}_0^2$ is a projection into the subspace of states having a different number of photons in both modes per each part. The subspace of such states is spanned by vectors $|k, l; m, n\rangle$ which are $a_1^{\dagger k} b_1^{\dagger l} a_2^{\dagger m} b_2^{\dagger n}|\Omega\rangle$ after normalization. The lower indices of creation operators denote measurement parties, $|\Omega\rangle$ is the vacuum state and $k \neq l$, $n \neq m$. Meanwhile, states having the same number of particles in both modes in one of the parties i.e. $k = l \vee n = m$ are in its orthogonal complement, to which we will refer as the *diagonal subspace*. As a consequence, the expectation value of such an operator for a generic state $|\psi\rangle$ is

$$\langle \hat{G}_0^1\hat{G}_0^2\rangle_\psi = 1 - P(d|\psi), \tag{11}$$

where $P(d|\psi)$ is the probability that we get as outcome an eigenvalue corresponding to a state belonging to the diagonal subspace when measuring $\hat{G}_0^1\hat{G}_0^2$ on the state $|\psi\rangle$. We can write the expectation value of the operator defined in equation (9) as a function of the probability appearing in equation (11):

$$\langle \hat{O}\rangle_\psi = 6 - 6P(d|\psi). \tag{12}$$

Thus, we can detect contextuality if:

$$P(d|\psi) < \frac{1}{3}, \tag{13}$$

as we have a violation of the inequality (10). A pitfall of this approach is that we lose state independence when considering the inequality violation. Again, the reason relies on the spectrum of our observables and, in particular, on the existence of the zero eigenvalue. However, we can still test the contextuality of a large class of states useful for the implementation of quantum optical technologies.

We stress that such construction to generalize the Peres–Mermin square using standard Stokes operators ($2\hat{S}_i$) and their normalized modification [17] fails to give satisfactory results due to the fact that both version of Stokes operators do not fulfill the anticommutaion relations of Pauli matrices.

3.2. Bright squeezed vacuum case

To substantiate our approach, we check when we observe a violation of the inequality in (10) considering as paradigmatic example the 2×2 bright squeezed vacuum (BSV). This state consists of two orthogonal modes per part and it can be written in the form:

$$\begin{aligned} |\psi_-\rangle &= \frac{1}{\cosh^2(\Gamma)} \sum_{n=0}^{\infty} \frac{\tanh^n(\Gamma)}{n!} (a_1^\dagger b_2^\dagger - a_2^\dagger b_1^\dagger)^n |\Omega\rangle \\ &= \frac{1}{\cosh^2(\Gamma)} \sum_{n=0}^{\infty} \sqrt{n+1}\, \tanh^n(\Gamma) |\psi^n\rangle, \end{aligned} \tag{14}$$

where $a_X^\dagger, b_X^\dagger (a_X, b_X)$ are the creation (annihilation) operators of the two orthogonal modes assigned to one of the two beams transmitted to the measurement part $X = 1, 2$. Furthermore, the parameter Γ denotes the amplification gain and it is related to the power of the coherent source impinging on the nonlinear crystal in the parametric down conversion process and

$$|\psi_-^n\rangle = \frac{1}{\sqrt{n+1}} \sum_{m=0}^{n} (-1)^m |(n-m)_{a_1}, m_{b_1}; m_{a_2}, (n-m)_{b_2}\rangle. \tag{15}$$

We note that when n is even, in the superposition in (15) there is always one term that belongs to the diagonal subspace, namely the one having $(n-m)_{a_x} = m_{b_x}$, where $x = 1, 2$. In contrast, for n odd, there are never terms from the diagonal subspace. Thus, by means of (14) the conditional probability of observing a result that can be associated with a state belonging to the diagonal subspace whenever a BSV state is prepared reads:

$$P(d|\mathrm{BSV}) = \frac{1}{\cosh^4(\Gamma)} \sum_{n=0}^{\infty} \tanh^{4n}(\Gamma) = \mathrm{sech}(2\Gamma). \tag{16}$$

From that follows that for $\Gamma > 0.89$ the BSV state does not allow a NCHV description, because in this range inequality (13) is fulfilled. In the limit of high pump power, namely for $\Gamma \to \infty$, we have $P(d|\mathrm{BSV}) = 0$. Thus, in the limit of mean photon number tending to infinity we obtain the same violation as in the case of qubits, which we shall address in the next section.

3.3. Qubit case

The original formulation of the Peres–Mermin square was in terms of qubit observables, so we can check if it is possible to retrieve the original Peres–Mermin square for qubits within the formalism we developed in section 2. Restricting to states with a single photon excitation per mode, we have a four dimensional subspace of a bipartite system (where the reduced state for each party has dimension two) and we recover the two qubits measurement scenario. As this subspace does not contain any diagonal states, we have the following:

$$\langle \hat{O} \rangle_{\mathrm{qubit}} = 6. \tag{17}$$

We recall that it is the same quantum expectation value as if one would construct analog of (9) using original Peres–Mermin square based on Pauli matrices [16]. Moreover, when the operators $\hat{G}_i^X$ act on states having one excitation per each beam X (note that each beam consists of two bosonic modes), they behave exactly as the standard Pauli matrices. Therefore, the original result is retrieved with its state independence and the original Peres–Mermin paradox can be obtained in our approach. Note that state independence is also retrieved for subspaces of states restricted to odd number of bosons per beam as it does not contain any diagonal state.

4. Entanglement

We address now if operators $\hat{G}_i$ can detect entanglement and whether they constitute advantage for this aim. To address the problem, we start proving that for any entanglement indicator written in the n-qubits of the form:

$$\hat{\mathcal{W}} = \sum_{s_1,\ldots,s_n=0}^{3} w_{s_1,\ldots,s_n} \bigotimes_{i=1}^{n} \hat{\sigma}^i_{s_i}, \tag{18}$$

exists a correspondence that maps the n-qubits entanglement indicator into a $2n$-bosonic modes entanglement indicator, that reads:

$$\hat{\mathcal{W}} \to \hat{\mathcal{W}}_G = \sum_{s_1,\ldots,s_n=0}^{3} w_{s_1,\ldots,s_n} \prod_{i=1}^{n} \hat{G}^i_{s_i}. \tag{19}$$

such that for any separable state ρ_{sep} the following relation holds

$$\text{Tr}\left\{\hat{W}_G \rho_{\text{sep}}\right\} = \langle \hat{\mathcal{W}}_G \rangle_{\text{sep}} \geqslant 0. \tag{20}$$

The proof proceeds in an analogous way to the one given in [18] for Stokes operators. To show how the mapping works we start with the case of $n = 2$. In order to prove (20) we have to show that for any mixed state ρ it is possible to find a density matrix $\hat{\mathcal{M}}_\rho$ describing a two-qubit state, which fulfill the following relation:

$$\frac{\langle \mathcal{W}_G \rangle_\rho}{\langle \hat{G}^1_0 \hat{G}^2_0 \rangle_\rho} = \text{Tr}\left[\hat{\mathcal{W}} \hat{\mathcal{M}}_\rho\right]. \tag{21}$$

We compute the expectation value of $\hat{G}^1_\eta \hat{G}^2_\nu$ on a pure state $|\phi\rangle$ using for the operators the expressions in equation (2), obtaining as a result:

$$\begin{aligned} \langle \hat{G}^1_\eta \hat{G}^2_\nu \rangle_{|\phi\rangle} &= \sum_{k,l=1}^{2} \sum_{n,m=1}^{2} \sigma^{kl}_\eta \sigma^{mn}_\nu \langle \Phi_{km} | \Phi_{ln} \rangle \\ &= \text{Tr}\left[\hat{\sigma}^1_\eta \otimes \hat{\sigma}^2_\nu \hat{M}_\phi\right], \end{aligned} \tag{22}$$

where $|\Phi_{ln}\rangle = \hat{V}^1_l \hat{V}^2_n |\phi\rangle$ and $\hat{V}^i_l$ is the lth element of the vector $\overrightarrow{V}$ that acts on the modes of the ith party as in (2). The matrix $\hat{M}_\phi$ has elements of the form $\langle \Phi_{km} | \Phi_{ln} \rangle$. This matrix is Gramian, therefore it is positive. Moreover, the following inequality:

$$0 < \text{Tr}\left[\hat{M}_\phi\right] = \langle \hat{G}^1_0 \hat{G}^2_0 \rangle_\phi \leqslant 1, \tag{23}$$

holds with the exception for cases where $|\phi\rangle$ is in the subspace of diagonal states. However, those cases are not interesting as the expectation value of $\hat{\mathcal{W}}_G$ is 0 and thus it cannot change the bound for separable states (20). We can now define the density matrix for a two-qubits system which fulfills (21) for a pure state $\rho = |\phi\rangle\langle\phi|$:

$$\hat{\mathcal{M}}_{|\phi\rangle} = \frac{\hat{M}_\phi}{\langle \hat{G}^1_0 \hat{G}^2_0 \rangle_\phi}. \tag{24}$$

For a mixed state ρ, which is a convex combination of states $|\phi_i\rangle\langle\phi_i|$, we get the following density matrix:

$$\hat{\mathcal{M}}_\rho = \frac{\sum_i p_i \hat{M}_{\phi_i}}{\sum_i p_i \ \text{Tr}\left[\hat{M}_{\phi_i}\right]}. \tag{25}$$

Consider a pure separable state of two-beam bosonic field $\left|\psi^{12}\right\rangle_{\text{sep}} = F^\dagger_1 F^\dagger_2 |\Omega\rangle$ where $F^\dagger_X$ is polynomial in the creation operators of the beam X. For such states, the following factorization occurs:

$${}_{\text{sep}}\langle \Phi_{km} | \Phi_{ln} \rangle_{\text{sep}} = \langle \Psi^1_k | \Psi^1_l \rangle \langle \Psi^2_m | \Psi^2_n \rangle, \tag{26}$$

where $\left|\Psi^X_l\right\rangle = \hat{V}^X_l F^\dagger_X |\Omega\rangle$. Thus, the matrix $\hat{M}_{\psi^{12}}$ factorizes into $\hat{M}^1_\psi \hat{M}^2_\psi$, where matrix elements of $\hat{M}^X_\psi$ are given by $\left\langle \Psi^X_k \middle| \Psi^X_l \right\rangle$. The matrix $\hat{M}^X_\psi$ after normalization is a well defined density matrix of qubit based on analogous arguments to those presented for $\hat{\mathcal{M}}_\rho$. Due to the factorization of the density matrix $\hat{\mathcal{M}}_\psi$, it describes a pure separable state in the two-qubit space, thus:

$$\langle \hat{\mathcal{W}} \rangle_{\hat{\mathcal{M}}_\psi} \geqslant 0. \tag{27}$$

As a mixed state is separable iff it is a convex combination of pure separable states, the matrix associated with such separable mixed state ρ' of the form (25) is a convex combination of two-qubit separable density matrices $\hat{\mathcal{M}}_{\psi_i}$. Using (27), we get that for any separable mixed state ρ' following inequality holds:

$$\langle \hat{\mathcal{W}} \rangle_{\hat{\mathcal{M}}_{\rho'}} = \frac{\sum_i p_i \ \mathrm{Tr}\left[\hat{M}_{\psi_i}\right] \langle \hat{\mathcal{W}} \rangle_{\hat{\mathcal{M}}_{\psi_i}}}{\sum_i p_i \ \mathrm{Tr}\left[\hat{M}_{\psi_i}\right]} \geqslant 0. \tag{28}$$

Thus, from the formula (21) we get:

$$\langle \hat{\mathcal{W}}_G \rangle_{\mathrm{sep}} = \langle \hat{\mathcal{W}}_G \rangle_{\rho'} \geqslant 0, \tag{29}$$

which is the condition for $\hat{\mathcal{W}}_G$ to be an entanglement indicator.

We check if such a mapping is true for any n-qubit case. Let us start extending it to the three qubits scenario. In such a case, any pure partially separable state of the three-beam bosonic field $\left|\psi^{123}\right\rangle$ can be written in factorized form, for example $\left|\psi^{123}\right\rangle_{\mathrm{sep}} = F_1^\dagger F_{23}^\dagger |\Omega\rangle$ where $F_{XY}^\dagger$ is a polynomial of creation operators associated with beams X and Y. Now we can analogously find the density matrix for three-qubit state $\hat{\mathcal{M}}_{\psi^{123}} = \hat{\mathcal{M}}_\psi^1 \hat{\mathcal{M}}_\psi^{23}$ which partially factorizes. Because the expectation value for any three-qubit entanglement indicator is non-negative for partially factorizable three-qubit density matrices, inequality (20) holds also for the three-beam case. Further extensions can be made following the previous arguments.

4.1. Entanglement of the bright GHZ state

Now we can adopt entanglement indicators for n-qubit states to examine the entanglement of states of bosonic fields. Let us recall the bright GHZ state (BGHZ), whose construction and entanglement has been presented in [19] for some range of amplification gain. This state is a generalization of two beam squeezed vacuum into the case of three beams. Current advancements in quantum optical experiments allow one to think about such generalizations to be feasible experimentally in the near future [20]. The usual methods used in the theoretical description of the generation of squeezed states, such as the parametric approximation turns out to be not well suited for this generalization. This is because the perturbation series in such approximation diverges. Still, using the Padé approximation one can find approximate convergent parametric description. The resulting state has the following form:

$$|\mathrm{BGHZ}\rangle = \sum_{k=0}^{\infty} \sum_{m=0}^{k} C_{k-m}(\Gamma) C_m(\Gamma) \times (\hat{a}_1^\dagger \hat{a}_2^\dagger \hat{a}_3^\dagger)^{k-m} (\hat{b}_1^\dagger \hat{b}_2^\dagger \hat{b}_3^\dagger)^m |\Omega\rangle, \tag{30}$$

where $\hat{a}_X^\dagger$, $\hat{b}_X^\dagger$ are creation operators in two orthogonal modes signed to an observer X and $C_m(\Gamma)$ are complex coefficients which can be obtained with the method from [19] for $\Gamma < 0.9$. In appendix D, we report how to construct the BGHZ state via the Padé approximation, and the full expressions of the coefficients $C_m(\Gamma)$. We can use our mapping $\sigma_i^1 \otimes \sigma_j^2 \otimes \sigma_k^3 \rightarrow \hat{G}_i^1 \hat{G}_j^2 \hat{G}_k^3$ to obtain a new entanglement indicator from the entanglement indicator tailored for GHZ state presented in [21]:

$$\mathcal{W} = \frac{3}{2} \hat{G}_0^1 \hat{G}_0^2 \hat{G}_0^3 - \hat{G}_1^1 \hat{G}_1^2 \hat{G}_1^3 - \frac{1}{2} (\hat{G}_0^1 \hat{G}_3^2 \hat{G}_3^3 + \hat{G}_3^1 \hat{G}_0^2 \hat{G}_3^3 + \hat{G}_3^1 \hat{G}_3^2 \hat{G}_0^3). \tag{31}$$

We use now this indicator to check the entanglement of the BGHZ state. It easy to see from equation (30) that it can be written as a superposition of states:

$$|\psi_{nm}\rangle = \frac{1}{\sqrt{2}} \left(|n_{a_1}, m_{b_1}; n_{a_2}, m_{b_2}; n_{a_3}, m_{b_3}\rangle + |m_{a_1}, n_{b_1}; m_{a_2}, n_{b_2}; m_{a_3}, n_{b_3}\rangle \right), \tag{32}$$

and diagonal states (with the same number of bosons in all modes) because states of superposition (32) have the same amplitudes in (30) independently from the exact form of coefficients $C_q(\Gamma)$. Note that the states $|\psi_{nm}\rangle$ are eigenstates of the operator $\hat{G}_1^1 \hat{G}_1^2 \hat{G}_1^3$ with eigenvalue 1. This is because the first element of the superposition (32) is turned into the second and vice versa under the action of $\hat{G}_1^1 \hat{G}_1^2 \hat{G}_1^3$. The action of such an operator on a diagonal state yields 0 and thus:

$$\langle \hat{G}_1^1 \hat{G}_1^2 \hat{G}_1^3 \rangle_{\mathrm{BGHZ}} = \langle \hat{G}_0^1 \hat{G}_0^2 \hat{G}_0^3 \rangle_{\mathrm{BGHZ}}. \tag{33}$$

An analogous equality is true for the last three terms of (31) because those operators acting on $|\psi_{nm}\rangle$ give $(-1)^2$ and for diagonal states we get 0. The term $\langle \hat{G}_0^1 \hat{G}_0^2 \hat{G}_0^3 \rangle_{\mathrm{BGHZ}}$ is simply the probability of observing result corresponding to non-diagonal states. As reported in appendix D the construction of BGHZ is valid only for the range of values of the amplification factor such as $0 < \Gamma < 0.9$. As a consequence:

$$\langle \mathcal{W} \rangle_{\mathrm{BGHZ}} = -\langle \hat{G}_0^1 \hat{G}_0^2 \hat{G}_0^3 \rangle_{\mathrm{BGHZ}} < 0. \tag{34}$$

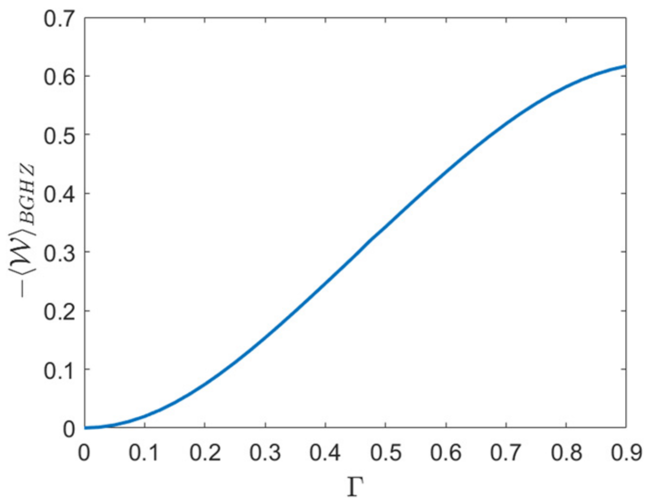

Figure 1. Expectation values of the entanglement indicator $\mathcal{W}$ for the BGHZ state versus Γ as in equation (31). From the curve one can observe that with increasing Γ the probability of measuring eigenvalues associated with non-diagonal states increases. The range of Γ is dictated by the fact that the method of calculating the probabilities of the BGHZ state has finite range of applicability [19].

The inequality in the preceeding equation is numerically confirmed and we report the result in figure 1. From that follows that for any Γ the state $|\text{BGHZ}\rangle$ is entangled. Figure 1 presents $-\langle \mathcal{W} \rangle_{\text{BGHZ}}$ versus Γ, for values of the amplification factor such that the $|\text{BGHZ}\rangle$ is well defined. We note that for terms of the BGHZ state with a fixed number of bosons per party k, the ratio between the number of diagonal states present in the superposition and the number of non-diagonal states drops to 0 also for even k. Moreover, because $\langle \hat{G}_0^1 \hat{G}_0^2 \hat{G}_0^3 \rangle_{\text{BGHZ}}$ increases when Γ increases, based on figure 1, the probability of observing eigenvalues corresponding to diagonal states decreases. This is valid at least in the range where we performed calculations. Thus, the probability distribution has no tendency to concentrate at the diagonal states with growing Γ as having corresponding eigenvalue 0 would indicate otherwise non-increasing pattern on the curve. However, as terms with greater photon numbers are generated by the same Hamiltonian such behaviour should be rather preserved also for $\Gamma > 0.9$. Thus, the probability of obtaining a result corresponding to a diagonal state, namely $P(d|\text{BGHZ}) = 1 - \langle \hat{G}_0^1 \hat{G}_0^2 \hat{G}_0^3 \rangle_{\text{BGHZ}}$, seems to decrease with growing Γ for any of its values and converge to 0, as the number of terms whose amplitudes have a relevant magnitude for the outcomes grows, while the diagonal terms become a minority among them and this effect is not countered by the concentration of probability distribution at the diagonal states. Thus, for $\Gamma \to \infty$ the expectation value of $\mathcal{W}$ should converge to the value of the three-qubit case, namely -1.

4.2. Necessary and sufficient condition to detect entanglement for a state of 2 × 2 modes using operators

A family of conditions for Pauli observables for two qubits which together form a necessary and sufficient condition for entanglement has been proposed in [22]. It was adapted to the case of Stokes operators in [18] using a mapping that has inspired our work. Using the analogous mapping between qubit conditions and the studied case, shown in (19), we can write a necessary and sufficient condition for *detecting* entanglement with the operators $\hat{G}_i$ for the two party scenario. It is

$$\langle \hat{G}_1^1 \hat{G}_1^2 + \hat{G}_2^1 \hat{G}_2^2 \rangle^2 + \langle \hat{G}_3^1 \hat{G}_0^2 + \hat{G}_0^1 \hat{G}_3^2 \rangle^2 \leqslant \langle \hat{G}_0^1 \hat{G}_0^2 + \hat{G}_3^1 \hat{G}_3^2 \rangle^2, \tag{35}$$

and the family of conditions which can be obtained from (35) by cyclically permuting the indices 1, 2, 3 of one party or both.

We shall employ this criterion to study the entanglement of the BSV state as defined in equation (14). It is easy to notice that $\hat{G}_0^1 \hat{G}_3^2 |\text{BSV}\rangle = -\hat{G}_3^1 \hat{G}_0^2 |\text{BSV}\rangle$ and $\hat{G}_0^1 \hat{G}_0^2 |\text{BSV}\rangle = -\hat{G}_3^1 \hat{G}_3^2 |\text{BSV}\rangle$. Thus, we have to consider the first term of the lhs of the inequality (35). One can also observe that $\hat{G}_1^1 \hat{G}_1^2 |\text{BSV}\rangle = \hat{G}_2^1 \hat{G}_2^2 |\text{BSV}\rangle$, because the sign part in $\hat{G}_2^1 \hat{G}_2^2$ cancels the signs coming from i^2 when acting on the BSV state. It turns out that:

$$\hat{G}_2^1 \hat{G}_2^2 |\psi^{2n+1}\rangle = -|\psi^{2n+1}\rangle, \tag{36}$$

$$\hat{G}_2^1 \hat{G}_2^2 |\psi^{2n}\rangle = \hat{G}_0^1 \hat{G}_0^2 |\psi^{2n}\rangle. \tag{37}$$

We calculate the first term in lhs of (35):

$$\langle \hat{G}_1^1\hat{G}_1^2 + \hat{G}_2^1\hat{G}_2^2\rangle^2 = 4\left[\sum_{n=0}^{\infty}\left(\frac{\tanh^{4n}\Gamma}{\cosh^4\Gamma} - \frac{\tanh^{4n+2}\Gamma}{\cosh^4\Gamma}\right) - \mathrm{sech}\,2\Gamma\right]^2$$
$$= 16\,\mathrm{sech}^4(2\Gamma)\sinh^4\Gamma. \tag{38}$$

This expression is always greater than zero for $\Gamma \neq 0$, therefore the operators $\hat{G}_i$ are able to detect entanglement for any $\Gamma > 0$ in agreement to what has been showed using Stokes operators [18].

5. Bell inequalities for the BGHZ state

In this section, we would like to show that operators $\hat{G}_i$ can allow for detecting Bell nonclassicality. Let us introduce the modification of operators $\hat{G}_i$:

$$\hat{G}_{i-} = \hat{G}_i - \sum_{n=0}^{\infty}|n,n\rangle\langle n,n|. \tag{39}$$

This modification effectively assigns the value -1 to the cases when an equal number of bosons is measured in both modes. The introduced modification of the operators makes them dichotomic observables as the Pauli matrices with the same spectrum of ± 1. Therefore, we can write the Mermin inequality [23] using the operators $\hat{G}_{i-}^j$:

$$|\langle G_{1-}^1(\lambda)G_{1-}^2(\lambda)G_{1-}^3(\lambda) - G_{1-}^1(\lambda)G_{2-}^2(\lambda)G_{2-}^3(\lambda) - G_{2-}^1(\lambda)G_{1-}^2(\lambda)G_{2-}^3(\lambda)$$
$$- G_{2-}^1(\lambda)G_{2-}^2(\lambda)G_{1-}^3(\lambda)\rangle_{\mathrm{LHV}}| \leqslant 2, \tag{40}$$

where λ is a local hidden variable and $G_{i-}^j(\lambda)$ are the local hidden values associated with the outcomes of measurement of operators $\hat{G}_{i-}^j$.

Now, we check whether it is possible to violate the inequality in (40) with the BGHZ state. As this state always has the same configuration of the number of bosons per any party, the operators $G_{i-}^1 G_{j-}^2 G_{k-}^3$ effectively reduce to:

$$\hat{G}_{i-}^1\hat{G}_{j-}^2\hat{G}_{k-}^3|\mathrm{BGHZ}_3\rangle = \left(\hat{G}_i^1\hat{G}_j^2\hat{G}_k^3 - \sum_{n=0}^{\infty}|\mathbf{n}\rangle\langle\mathbf{n}|\right)|\mathrm{BGHZ}_3\rangle, \tag{41}$$

where $|\mathbf{n}\rangle$ is the state having the same number of particles, n, in all the modes. Using (33) one can find that:

$$\langle \hat{G}_{1-}^1\hat{G}_{1-}^2\hat{G}_{1-}^3\rangle_{\mathrm{BGHZ}} = 1 - 2P(d|\mathrm{BGHZ}), \tag{42}$$

where $P(d|\mathrm{BGHZ}) = 1 - \langle \hat{G}_0^1\hat{G}_0^2\hat{G}_0^3\rangle_{\mathrm{BGHZ}}$. We have used here the fact that only diagonal states contained in BGHZ are states with the same number of photons in all modes. One can also see that:

$$\langle \hat{G}_1^1\hat{G}_2^2\hat{G}_2^3\rangle_{\mathrm{BGHZ}} = \mathrm{i}^2\langle \hat{G}_1^1\hat{G}_1^2\hat{G}_1^3\rangle_{\mathrm{BGHZ}}$$
$$= -\langle \hat{G}_0^1\hat{G}_0^2\hat{G}_0^3\rangle_{\mathrm{BGHZ}}, \tag{43}$$

and from that follows:

$$\langle \hat{G}_{1-}^1\hat{G}_{2-}^2\hat{G}_{2-}^3\rangle_{\mathrm{BGHZ}} = -\langle \hat{G}_0^1\hat{G}_0^2\hat{G}_0^3\rangle_{\mathrm{BGHZ}} - P(d|\mathrm{BGHZ}) = -1. \tag{44}$$

Analogous results hold for last two terms of (40), hence for the BGHZ state we get:

$$4 - 2P(d|\mathrm{BGHZ}) \leqslant 2. \tag{45}$$

This inequality is violated for any $\Gamma > 0$ because $2P(d|\mathrm{BGHZ}) < 2$ and as it was discussed in section 4.1, and for $\Gamma \to \infty$ we retrieve the three-qubit case. This situation is opposite to the case where for constructing Mermin inequality normalized Stokes operators were used [19]. This is in the sense that for normalized Stokes operators the range of violation is finite ($\Gamma < 0.77$) and the strongest violation is obtained for low values of Γ.

The introduced modification allowed for violation in the whole range of Γ. Without this modification, one would get:

$$4 - 4P(d|\text{BGHZ}) \leqslant 2, \tag{46}$$

which is not violated for small Γ. However, in the limit of high values of Γ, the behaviour of this inequality does not deviate significantly from (45).

6. Conclusions

The quantification of nonclassical properties of bosonic fields has always played a pivotal role for the development of quantum technologies. Nowadays, the experimental techniques for counting the number of particles present in a bosonic mode open new avenues to detect and quantify several nonclassical resources [24–27]. However, special care must be taken when generalizing some concepts formulated for fixed number of particles, to situations inherently involving undefined particle numbers, see e.g. discussion in [28–32]. Here, we introduce a set of new Stokes-like observables for two modes of a bosonic field, which turns out to be a representation of $\mathfrak{su}(2)$ algebra. Using these operators we construct a generalization of the Peres–Mermin square for a four-modes bosonic field, which allows to observe contextuality for states with an undefined number of particles. This shows that contextuality is not only a phenomenon observable for low dimensional quantum systems, and supersedes the approaches relying on the phase-space formalism [12, 13]. Particle-counting detection allows to extend the results to massive bosonic fields beyond the optical ones. Our generalization is not state independent, and the restriction to a single-boson excitation per party retrieves the original formulation of the Peres–Mermin square.

We also present a mapping of n-qubit entanglement indicators to entanglement indicators for bosonic fields, which uses the Pauli-like observables, which enter our Peres–Mermin square. This allows us e.g. to show that a BGHZ state, a parametric process involving multiple emission to triple of polarization correlated photons, is entangled for any brightness. We also provide a necessary and sufficient criterion for four mode states, which allows to detect entanglement with the Pauli-like observables. Its efficiency is shown for the 2×2 BSV state. Lastly, we show a violation of the Bell inequality, based on the operators that we have introduced, for the BGHZ state in the whole range of the amplification gain. For all the three studied quantifiers of the nonclassicalicality of a field, we have observed that the results obtained for qubits can be recovered once one considers states with one particle in each beam heading to each detection station. Note that, the previous generalizations of the Pauli formalism in an optical context, in form of standard Stokes operators, and normalized Stokes operators, see e.g. [33], do not allow to generalize the Peres–Mermin construction.

As a final remark, we address an open question that arises from our results. How can be experimentally realized a measurement of such observables? Conceptually, the measurement of $\hat{G}_3$, the last operator from proposed set, does not pose any difficulty, however measuring the another two operators seems to involve a highly nontrivial experimental procedure. This question may be of great significance for observing nonclassical aspects of quantum optical fields for macroscopic states as those observables seem to be optimal for this kind of states. Thus, this construction can stimulate advancements in experimental methods in quantum optics. Once it will be achieved, we forecast that such a strategy can also be fruitful to quantify the nonclassicality of other bosonic fields, such as many-body systems of massive particle composing Bose Einstein condensate [27]. Another interesting task is to operationally construct a generalization of the proposed scheme to also cover optical realizations of generalized Gell–Mann observables. This would involve multiport beamsplitters [34].

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Data availability statement

No new data were created or analysed in this study.

Appendix A. Anticomutation and commutation relations

Firstly, let us check if $\{\hat{G}_1, \hat{G}_3\} = 0$. This can be verified by acting with $\hat{G}_1\hat{G}_3$ and $\hat{G}_3\hat{G}_1$ on the basis vectors $|n, m\rangle$ and $|m, n\rangle$ for $n > m$. Knowing that $\hat{G}_1$ swaps modes and that states $|n, m\rangle(|m, n\rangle)$ are eigenvectors of $\hat{G}_3$ with eigenvalue $1(-1)$ we get for $|n, m\rangle$:

$$\hat{G}_1\hat{G}_3|n, m\rangle = \hat{G}_1|n, m\rangle = |m, n\rangle,$$
$$\hat{G}_3\hat{G}_1|n, m\rangle = \hat{G}_3|m, n\rangle = -|m, n\rangle,$$

and for $|mn\rangle$

$$\hat{G}_1\hat{G}_3|m, n\rangle = -\hat{G}_1|m, n\rangle = -|n, m\rangle,$$
$$\hat{G}_3\hat{G}_1|m, n\rangle = \hat{G}_3|n, m\rangle = |n, m\rangle.$$

Because diagonal states have eigenvalue 0 for both those operators, we have $\hat{G}_3\hat{G}_1 = -\hat{G}_1\hat{G}_3$ and thus, the anticommutation relation is fulfilled.

Now let us check if $\{\hat{G}_1, \hat{G}_2\} = 0$. One can observe that $\hat{G}_2 = -\mathrm{i}\hat{G}_3\hat{G}_1$ and so we have:

$$\hat{G}_2\hat{G}_1 = -\mathrm{i}\hat{G}_3\hat{G}_1\hat{G}_1 = -\mathrm{i}\hat{G}_3\hat{G}_0 = -i\hat{G}_3,$$
$$\hat{G}_1\hat{G}_2 = -\mathrm{i}\hat{G}_1\hat{G}_3\hat{G}_1 = -\mathrm{i}\hat{G}_1(-\hat{G}_1\hat{G}_3)$$
$$= \mathrm{i}\hat{G}_0\hat{G}_3 = \mathrm{i}\hat{G}_0\hat{G}_3.$$

In the previous expression, we have used the fact that $\hat{G}_1^2 = \hat{G}_0$ which is easily seen form the fact that flipping modes two times does not change a state. We have also used that $\hat{G}_0\hat{G}_i = \hat{G}_i\hat{G}_0 = \hat{G}_i$ which follows from that $\hat{G}_0$ has a common zero eigenvalue for diagonal states with any $\hat{G}_i$ and it has eigenvalue 1 for other states (this also shows that $\hat{G}_0$ commutes with any $\hat{G}_i$). As a result, we obtain $\{\hat{G}_1, \hat{G}_2\} = 0$.

Now we check if $\{\hat{G}_2, \hat{G}_3\} = 0$. Using the fact that $\hat{G}_3^2 = \hat{G}_0$ we get:

$$\hat{G}_2\hat{G}_3 = -\mathrm{i}\hat{G}_3\hat{G}_1\hat{G}_3 = -\mathrm{i}\hat{G}_3(-\hat{G}_3\hat{G}_1) = \mathrm{i}\hat{G}_0\hat{G}_1,$$
$$\hat{G}_3\hat{G}_2 = -\mathrm{i}\hat{G}_3\hat{G}_3\hat{G}_1 = -\mathrm{i}\hat{G}_0\hat{G}_1 = -\mathrm{i}\hat{G}_1.$$

Thus, the anticommutation relation under consideration holds.

Lastly, we check if $\hat{G}_2^2 = \hat{G}_0$:

$$\hat{G}_2^2 = -\mathrm{i}\hat{G}_3\hat{G}_1(-\mathrm{i}\hat{G}_3\hat{G}_1) = -\hat{G}_3\hat{G}_1\hat{G}_3\hat{G}_1$$
$$= \hat{G}_3\hat{G}_3\hat{G}_1\hat{G}_1 = \hat{G}_0^2 = \hat{G}_0.$$

Taking all these relations together, we have:

$$\{\hat{G}_i, \hat{G}_j\} = 2\delta_{ij}\hat{G}_0.$$

Let us now check the commutation relations. We start with $[\hat{G}_3, \hat{G}_1]$. Using the anticomutation relations, previously proved, we have:

$$\hat{G}_3\hat{G}_1 - \hat{G}_1\hat{G}_3 = 2\hat{G}_3\hat{G}_1 = 2\mathrm{i}\hat{G}_2, \tag{A1}$$

where the last equality follows from $\hat{G}_2 = -\mathrm{i}\hat{G}_3\hat{G}_1$. In case of $[\hat{G}_1, \hat{G}_2]$ we have:

$$\begin{aligned}\hat{G}_1\hat{G}_2 - \hat{G}_2\hat{G}_1 &= -2\hat{G}_2\hat{G}_1\\ &= 2\mathrm{i}\hat{G}_3\hat{G}_1\hat{G}_1 = 2\mathrm{i}\hat{G}_3.\end{aligned} \tag{A2}$$

Finally, for $[\hat{G}_2, \hat{G}_3]$ we have:

$$\begin{aligned}\hat{G}_2\hat{G}_3 - \hat{G}_3\hat{G}_2 &= -2\hat{G}_3\hat{G}_2\\ &= 2\mathrm{i}\hat{G}_3\hat{G}_3\hat{G}_1 = 2\mathrm{i}\hat{G}_1.\end{aligned} \tag{A3}$$

Thus, the commutation relations for the set of operators $\hat{G}_i$ are as follows:

$$[\hat{G}_i, \hat{G}_j] = 2\mathrm{i}\epsilon_{ijk}\hat{G}_k \tag{A4}$$

Adding the anticommutation relation and commutation relation, we obtain:

$$(\hat{G}_i\hat{G}_j - \hat{G}_j\hat{G}_i) + (\hat{G}_i\hat{G}_j + \hat{G}_j\hat{G}_i) = 2\hat{G}_i\hat{G}_j = 2\mathrm{i}\epsilon_{ijk}\hat{G}_k + 2\delta_{ij}\hat{G}_0,$$

and from this follows an analogous relation as for the Pauli matrices:

$$\hat{G}_i\hat{G}_j = \delta_{ij}\hat{G}_0 + \mathrm{i}\epsilon_{ijk}\hat{G}_k. \tag{A5}$$

Appendix B. Spectrum of operators

We can characterize the set of eigenvectors for operators $\hat{G}_i$. In the case of $\hat{G}_1$ we have:

$$\begin{aligned} &\frac{1}{\sqrt{2}}(|n,m\rangle + |m,n\rangle) && \text{for eigenvalue } 1,\\ &\frac{1}{\sqrt{2}}(|n,m\rangle - |m,n\rangle) && \text{for eigenvalue } -1,\\ &|n,n\rangle && \text{for eigenvalue } 0. \end{aligned}$$

Let us now assume that $n > m$. For the operator $\hat{G}_2$ we obtain:

$$\begin{aligned} &\frac{1}{\sqrt{2}}(|n,m\rangle + \mathrm{i}|m,n\rangle) && \text{for eigenvalue } 1\\ &\frac{1}{\sqrt{2}}(|n,m\rangle - \mathrm{i}|m,n\rangle) && \text{for eigenvalue } -1,\\ &|n,n\rangle && \text{for eigenvalue } 0. \end{aligned}$$

Finally, for the operator $\hat{G}_3$ we have:

$$\begin{aligned} &|n,m\rangle && \text{for eigenvalue } 1\,,\\ &|m,n\rangle && \text{for eigenvalue } -1,\\ &|n,n\rangle && \text{for eigenvalue } 0. \end{aligned}$$

Considering the three basis vectors $|n,n\rangle, |n,m\rangle, |m,n\rangle$ we can write the three orthonormal eigenvectors for any of the operators, we can sum up that this set of eigenvectors characterizes all eigenvectors of $\hat{G}_i$ and that the spectrum of operators $\hat{G}_i$ is $\pm 1, 0$.

Appendix C. Unitary transformation of modes

It can be shown that the set of operators $\hat{S}_i = \frac{1}{2}A^\dagger\sigma_i A$ after unitary transformation, which is equivalent to cyclic permutation of the basis, will result in an equivalent set of operators only changing their labelling. However, the same is not true for the set of operators $\hat{G}_i$

To see that, let us consider two orthonormal mutually unbiased polarization bases $\{\mathrm{H},\ \mathrm{V}\}$ (horizontal, vertical) and $\{\mathrm{D},\ \mathrm{A}\}$ (diagonal, anti-diagonal) and their creation operators, respectively: $a_\mathrm{H}^\dagger, b_\mathrm{V}^\dagger$ and $a_\mathrm{D}^\dagger b_\mathrm{A}^\dagger$. If one writes the $\hat{S}_3^{(\mathrm{D})}$ operator based on $a_\mathrm{D}^\dagger, b_\mathrm{A}^\dagger$ one expects that this operator rewritten in the $\{\mathrm{H},\ \mathrm{V}\}$ basis will coincide with the operator $\hat{S}_1^{(\mathrm{H})}$ based on $a_\mathrm{H}^\dagger, b_\mathrm{V}^\dagger$. We show that this is not true for operators $\hat{G}_i$ on the basis of a counterexample.

As $\hat{G}_i$ and $\hat{S}_i$ coincide in the one photon subspace up to coefficient, the first nontrivial counterexample can be shown in the two-photon subspace. Let us consider $\hat{G}_3^{(\mathrm{D})}$ restricted to two photon subspace:

$$\hat{G}_3^{(\mathrm{D}|2)} := |2_\mathrm{D}, 0_\mathrm{A}\rangle\langle 2_\mathrm{D}, 0_\mathrm{A}| - |0_D, 2_\mathrm{A}\rangle\langle 0_\mathrm{D}, 2_\mathrm{A}|. \tag{C1}$$

After rewriting this operator in $\{\mathrm{H},\ \mathrm{V}\}$ basis we obtain:

$$\hat{G}_3^{(\mathrm{D}|2)} = -\frac{1}{\sqrt{2}}\big(|2_\mathrm{H}, 0_\mathrm{V}\rangle\langle 1_\mathrm{H}, 1_\mathrm{V}| + |0_\mathrm{H}, 2_\mathrm{V}\rangle\langle 1_\mathrm{H}, 1_\mathrm{V}| + |1_\mathrm{H}, 1_\mathrm{V}\rangle\langle 2_\mathrm{H}, 0_\mathrm{V}| + |1_\mathrm{H}, 1_\mathrm{V}\rangle\langle 0_\mathrm{H}, 2_\mathrm{V}|\big). \tag{C2}$$

As this operator does not coincide with $\hat{G}_1^{(\mathrm{H}|2)}$, the operators $\hat{G}_i$ do not share the considered property with the operators $\hat{S}_i$.

Appendix D. Bright GHZ state

Here we briefly recall construction of BGHZ state.

Consider a Hamiltonian of the following form:

$$\hat{H}^a = \gamma \hat{a}_1^\dagger \hat{a}_2^\dagger \hat{a}_3^\dagger + \text{h.c.} \tag{D1}$$

where $\hat{a}_i^\dagger$ stand for creation operators in three orthogonal modes. This interaction Hamiltonian is a parametric approximation, essentially replacement of the quantum description of the laser field by a classical amplitude of electromagnetic field, of the process of down conversion of photons from the pumping laser field (described by the parameter γ) into triples of photons. However, this parametric approximation does not lead to a normalizable state. If one treats seriously H^a than straight ahead calculation of the evolution of the vacuum state leads to the following:

$$|\Sigma^n\rangle = \mathrm{e}^{\mathrm{i}H^a t}|\Omega\rangle, \tag{D2}$$

what after a series expansion could be put as:

$$|\Sigma^n\rangle = \sum_{k=0}^{\infty} c_k (\hat{a}_1^\dagger \hat{a}_2^\dagger \hat{a}_3^\dagger)^k |\Omega\rangle. \tag{D3}$$

If one puts $\Gamma = t\gamma$, we have the following formal recurrence:

$$c_k = \sum_{l=0}^{\infty} \frac{(\mathrm{i}\Gamma)^{k+2l}}{(k+2l)!} P_{k+2l}^k, \tag{D4}$$

where P_l^k obey the relation: $P_l^k = P_{l-1}^{k-1} + (k+1)^3 P_{l-1}^{k+1}$ with $P_l^k = 0$ if $k > l$ and $P_k^k = 1$. However, such approach to the parametric approximation fails to properly describe a generated state as series (D4) do not converge for any $\Gamma > 0$, as for the case of the problem of the generalization of squeezing with Hamiltonians proportional to $(a^\dagger)^n + \text{h.c.}$ for $n > 2$ [35]. However, one can obtain approximate parametric description for $\Gamma < 0.9$ of such state by using Padé approximants [19]. In such a case we have:

$$|\Sigma^n\rangle = \sum_{k=0}^{\infty} C_k(\Gamma) (\hat{a}_1^\dagger \hat{a}_2^\dagger \hat{a}_3^\dagger)^k |\Omega\rangle, \tag{D5}$$

with $C_k(\Gamma)$ being rational functions (Padé approximants of degree $[N/M]$):

$$C_k(\Gamma) = \frac{\sum_{n=0}^{N} X_n^k (\mathrm{i}\Gamma)^n}{\sum_{m=0}^{M} Y_m^k (\mathrm{i}\Gamma)^m}, \tag{D6}$$

with coefficients X_n^k, Y_m^k such that the first $(N + M + 1)$ terms of the Taylor series expansion of $C_k(\Gamma)$ match the first $(N + M + 1)$ terms of (D4). For the calculations in this paper we use degree $[40/40]$.

The BGHZ state involving modes a and b could be thought as arising from the Hamiltonian:

$$\hat{H} = \hat{H}^a + \hat{H}^b, \tag{D7}$$

where $\hat{H}^b = \gamma \hat{b}_1^\dagger \hat{b}_2^\dagger \hat{b}_3^\dagger + \text{h.c.}$. Due to the fact that $\hat{H}^a$ commutes with $\hat{H}^b$, down conversions to modes a_i are independent from conversions to modes b_i i.e.:

$$\mathrm{e}^{\mathrm{i}(\hat{H}^a + \hat{H}^b)t} = \mathrm{e}^{\mathrm{i}\hat{H}^a t}\, \mathrm{e}^{\mathrm{i}\hat{H}^b t}. \tag{D8}$$

We have the same situation in the case of their not-parametrically approximated versions with quantum operators describing the laser field, provided the two processes are linked with annihilation of pump photons of orthogonal polarizations. That is, if the pump field annihilation operators can be denoted as $\hat{c}$ and $\hat{c}_\perp$, the fully quantum interaction Hamiltonian in proportional to $\hat{c}\hat{b}_1^\dagger \hat{b}_2^\dagger \hat{b}_3^\dagger + \hat{c}_\perp \hat{a}_1^\dagger \hat{a}_2^\dagger \hat{a}_3^\dagger + \text{h.c.}$. Thus the approximated structure of BGHZ state can be put in the form as in equation (30).

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PAPER

Generalization of Gisin's theorem to quantum fields

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Abstract

We generalize Gisin's theorem on the relation between the entanglement of pure states and Bell non-classicality to the case of mode entanglement of separated groups of modes of quantum fields extending the theorem to cover also states with undefined particle number. We show that *any* pure state of the field which contains entanglement between two groups of separated modes violates some Clauser–Horne (CH) inequality. In order to construct the observables leading to a violation in the first step, we show an isomorphism between the Fock space built from a single-particle space involving two separated groups of modes and a tensor product of two abstract separable Hilbert spaces spanned by formal monomials of creation operators. In the second step, we perform a Schmidt decomposition of a given entangled state mapped to this tensor product space and then we map back the obtained Schmidt decomposition to the original Fock space of the system under consideration. Such obtained Schmidt decomposition in Fock space allows for construction of observables leading to a violation of the CH inequality. We also show that our generalization of Gisin's theorem holds for the case of states on non-separable Hilbert spaces, which physically represent states with actually infinite number of particles. Such states emerge, for example, in the discussion of quantum phase transitions. Finally, we discuss the experimental feasibility of constructed Bell test and provide a necessary condition for realizability of this test within the realm of passive linear optics.

1. Introduction

The superposition principle is one of the quantum phenomena that has impacted our fundamental understanding of nature the most. Especially, the concept of entanglement, which emerges from the superposition principle, exposes the failure of classical intuitions like local realism presented in the EPR paradox [1] and discussed in the entire Bell-inequalities literature [2–7]. The introduction of Bell inequalities [8] allowed for a direct proof of the incompatibility of quantum mechanics with local hidden variable (LHV) probabilistic models giving rise to the phenomenon of Bell non-classicality. Those theoretical predictions were then experimentally tested confirming the predictions of quantum mechanics [9, 10].

This confirmation, however, does not answer the question whether Bell non-classicality is a general feature of pure entangled states. Especially the question of whether Bell non-classicality can also be revealed by arbitrarily weakly entangled states. The first step in answering this question was formulation of Gisin's theorem [11] which states that any entangled *two-qubit* state violates some Bell inequality. This was followed by an extension to a higher number of systems [12] with a recent complement [13]. The theorem was further generalized to an arbitrarily large number of particles and the arbitrary dimension of single-particle Hilbert spaces [14, 15]. However, those generalizations do not provide a full answer to the question, since the analysis therein is performed in terms of first quantization, which requires fixing the number of particles. However, it is known that entanglement also exists for states with an undefined number of particles [16–19], which requires the second quantization for its description. Therefore, the natural framework for treating this problem is provided by quantum field theory which more closely describes nature and allows for better insight into the foundations of physical theories.

In this paper, we present a generalization of Gisin's theorem to an arbitrary entangled pure state in quantum field theory. We present the construction of the Schmidt decomposition for multimode states in the Fock space, which then leads to the construction of the state-specific Clauser–Horne (CH) inequality [20] violated by the given arbitrary entangled state. We show that our generalization holds also in the case of a non-separable extension of the Fock space (which includes states with an infinite number of particles) in terms of entanglement of quasi-particles. Finally, we show the necessary condition for Bell non-classicality to be observed by projective particle-number-non-mixing measurements realizable within passive linear optics. This condition allows for determining whether the homodyne measurement or another non-projective POVM-type measurement is necessary to demonstrate Bell non-classicality for a given mode-entangled state.

2. Preliminaries

In order to consider entanglement, one has to introduce the state space of the theory. Let us briefly recall the construction of the state space in the first and second quantizations.

2.1. First quantization state space and entanglement

The state of a single particle in the first quantization is specified by a normalized vector $|\psi\rangle$ in the single-particle Hilbert space $\mathcal{H}$. This Hilbert space, in general, is isomorphic to the space associated with wave functions i.e. space of square-integrable functions $L^2(\mathcal{M})$ on a given d-dimensional manifold $\mathcal{M}$ in which the particle lives or to its subspace determined by the evolution equations. Therefore, as $L^2(\mathcal{M})$ is separable Hilbert space $\mathcal{H}$ is also separable, which is equivalent to saying that one can construct a countable basis in $\mathcal{H}$. Then, the state space of two distinct particles is given by the tensor product of the corresponding single-particle spaces $\mathcal{H}_1 \otimes \mathcal{H}_2$. Such a construction gives rise to a natural division of the system into two subsystems among which the entanglement can be considered. In general, in the case of two separable Hilbert spaces constructed by means of a tensor product, one can decompose any state $|\psi_{12}\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ in terms of Schmidt decomposition [21]:

$$|\psi_{12}\rangle = \sum_t \lambda_t |\phi_t\rangle_1 \otimes |\varphi_t\rangle_2, \tag{1}$$

with coefficients $\lambda_t \geqslant 0$ which fulfill $\sum_t |\lambda_t|^2 = 1$, and vectors $|\phi_t\rangle_1 \in \mathcal{H}_1$, $|\varphi_t\rangle_2 \in \mathcal{H}_2$ forming sets of orthonormal vectors i.e. $\langle \phi_t|\phi_{t'}\rangle_1 = \langle \varphi_t|\varphi_{t'}\rangle_2 = \delta_{t,t'}$ where $\delta_{t,t'}$ stands for the Kronecker delta. Importantly, this decomposition is unique up to the choice of phase of vectors $|\phi_t\rangle_1$, $|\varphi_t\rangle_2$. Upon this decomposition, one can uniquely determine whether a state is entangled or separable, since for any separable state $\exists! \lambda_t \neq 0$. The number r of nonzero λ_t's is referred to as the Schmidt rank of the state.

2.2. Second quantization state space and entanglement

In quantum field theory, the state space for a given field is given by the Fock space. This space is constructed upon a single-particle Hilbert space $\mathcal{H}$ as the direct sum of the symmetrized or antisymmetrized tensor product of arbitrarily large number of copies of $\mathcal{H}$:

$$\mathcal{F}(\mathcal{H})_{+(-)} = \bigoplus_{n=0}^{\infty} \mathcal{S}_{+(-)}\left(\mathcal{H}^{\otimes n}\right), \tag{2}$$

where $\mathcal{S}_+$ stands for symmetrization and $\mathcal{S}_-$ for antisymmetrization. The operation $\mathcal{S}_q$ accounts for the indistinguishability of particles of given species with $q = +$ for bosons and $q = -$ for fermions. The infinite direct sum allows for a description of an arbitrary number of particles. Note that this space, in fact, does not contain states with an infinite number of particles, since all well-defined states have always zero probability to find an infinite number of quanta. In this space, one introduces the creation $\hat{a}_i^\dagger$ and annihilation $\hat{a}_i$ operators, which add or remove a single particle in the mode a_i. These operators fulfill canonical commutation or anticommutation relations for bosons and fermions, respectively:

$$\left[\hat{a}_i, \hat{a}_j^\dagger\right] = \delta_{i,j},\ \left[\hat{a}_i, \hat{a}_j\right] = \left[\hat{a}_i^\dagger, \hat{a}_j^\dagger\right] = 0, \tag{3}$$

$$\left\{\hat{a}_i, \hat{a}_j^\dagger\right\} = \delta_{i,j},\ \left\{\hat{a}_i, \hat{a}_j\right\} = \left\{\hat{a}_i^\dagger, \hat{a}_j^\dagger\right\} = 0. \tag{4}$$

Note that the modes correspond to the choice of orthonormal basis vectors in a single-particle space $\mathcal{H}$, and thus the construction of the creation and annihilation operators is not unique. The canonical basis in $\mathcal{F}(\mathcal{H})_q$

is the Fock basis (occupation-number basis) and it can be always constructed from the vacuum state $|\Omega\rangle$, defined by the relation $\hat{a}_i|\Omega\rangle = 0$, which contains zero quanta, using creation operators $\hat{a}_i^\dagger$:

$$|n_1, n_2, \ldots\rangle = \frac{\left(\hat{a}_1^\dagger\right)^{n_1}\left(\hat{a}_2^\dagger\right)^{n_2}\ldots}{\sqrt{n_1!n_2!\ldots}}|\Omega\rangle, \tag{5}$$

where $\sum_i n_i < \infty$ for bosons, and for fermions $n_i \in \{0,1\}$. Note that the Fock space is separable, as the countable basis of $\mathcal{H}$ induces a countable number of modes, and there is only a finite number of quanta in those modes.

Different types of entanglement were considered in the Fock space [22–24]. One of them is the concept of entanglement of indistinguishable particles emerging from the symmetrization procedure in Fock space construction. However, let us comment that this type of entanglement is not directly accessible by nature and rather seems to be a mathematical artifact of the construction of the Fock space. This is because one cannot build local observables without some effective distinguishability. As an example, consider the following state of two indistinguishable bosons in two modes

$$|1,1\rangle = \frac{1}{\sqrt{2}}\left(|a_1\rangle_1|a_2\rangle_2 + |a_2\rangle_1|a_1\rangle_2\right), \tag{6}$$

where kets indices mark the corresponding single-particle Hilbert spaces. However, those indices are not accessible as the environment has to couple to all single-particle Hilbert spaces in the same way due to indistinguishability. However, this does not preclude the possibility of utilizing indistinguishability of particles to obtain conditional multipartite interference effects, see e.g. [25–27], which by nature do not demand addressing of inaccessible particle labels.

The entanglement of quantum fields that can be directly observed is the mode entanglement. In this approach to entanglement, the effective distinguishability is obtained due to the orthogonality of modes, which allows for probing their properties separately by construction of mode-local observables. Let us divide modes emerging from some single-particle Hilbert space $\mathcal{H}_{\mathcal{AB}}$ into two families $\{a_i\}$, $\{b_l\}$ (where i and l are countable indices). A state $|\psi_{a,b}\rangle$ in the Fock space $\mathcal{F}(\mathcal{H}_{\mathcal{AB}})_q$ is separable iff:

$$|\psi_{a,b}\rangle = F\left(a_i^\dagger\right)G\left(b_l^\dagger\right)|\Omega\rangle, \tag{7}$$

where $F(a_i^\dagger)$, $G(b_l^\dagger)$ are some polynomials of the creation operators in modes $\{a_i\}$, $\{b_l\}$ respectively.

3. Schmidt decomposition in Fock space

Let us start with an explicit construction of the Schmidt decomposition in Fock space. Note that construction of the Fock space (2) does not have a natural form of a tensor product of two Hilbert spaces $\mathcal{H}_1 \otimes \mathcal{H}_2$ which is used in a standard Schmidt decomposition. Therefore, as a first step, we prove that the Fock space $\mathcal{F}(\mathcal{H}_{\mathcal{AB}})_q$ is isomorphic to the tensor product of two abstract separable Hilbert spaces $\mathcal{H}_{\mathcal{A}} \otimes \mathcal{H}_{\mathcal{B}}$. Note that in the following, the type of field determined by q will not play any role, and the result will be valid for both.

Let us denote by $\{\vec{n}^j\}_{j=1}^\infty$ and $\{\vec{m}^{j'}\}_{j'=1}^\infty$ sets of all vectors of the form $\vec{n}^j = (n_1^j, n_2^j, \ldots)$ and $\vec{m}^{j'} = (m_1^{j'}, m_2^{j'}, \ldots)$ where $\sum_{i=1}^{\overline{\{a_i\}}} n_i^j < \infty$, $\sum_{l=1}^{\overline{\{b_l\}}} m_l^{j'} < \infty$. These two sets describe all possible distributions of a finite number of particles among two groups of orthogonal modes $\{a_i\}$ and $\{b_l\}$, which can in principle contain an infinite (though countable) number of modes. Note that an arbitrary element of an occupation-number basis of $\mathcal{F}(\mathcal{H}_{\mathcal{AB}})$ can be represented by two integer indices j, j' as follows:

$$|j,j'\rangle = |\vec{n}^j;\vec{m}^{j'}\rangle = \frac{1}{\mathcal{N}_a\mathcal{N}_b}\prod_i\left(\hat{a}_i^\dagger\right)^{n_i^j}\prod_l\left(\hat{b}_l^\dagger\right)^{m_l^{j'}}|\Omega\rangle = f\left(a_i^\dagger, j\right)g\left(b_l^\dagger, j'\right)|\Omega\rangle, \tag{8}$$

in which $\mathcal{N}_{a/b}$ is a normalization factor, and $f(a_i^\dagger, j)$, $g(b_l^\dagger, j')$ denote suitable monomials of creation operators in modes $\{a_i\}$, $\{b_l\}$ respectively. Under such constraints $\{|j,j'\rangle\}_{jj'}$ is a countable orthogonal basis of $\mathcal{F}(\mathcal{H}_{\mathcal{AB}})$ with natural inner product:

$$\langle jj'|kk'\rangle = \delta_{\vec{n}^j,\vec{n}^k}\delta_{\vec{m}^{j'},\vec{m}^{k'}} = \delta_{j,k}\delta_{j',k'}, \tag{9}$$

in which the deltas are equal to one iff the two vectors are equal and zero otherwise.

Since the monomials $f(a_i^\dagger, j)$, $g(b_l^\dagger, j')$ are uniquely defined via indices j, j', we can construct two Hilbert spaces $\mathcal{H}_A$, $\mathcal{H}_B$ over scalars $\mathbb{C}$ as spanned by abstract orthogonal basis vectors $\tilde{f}(j)$, $\tilde{g}(j')$ respectively, with scalar products specified by:

$$\langle \tilde{f}(j) | \tilde{f}(k) \rangle = \delta_{j,k}$$
$$\langle \tilde{g}(j') | \tilde{g}(k') \rangle = \delta_{j',k'}. \tag{10}$$

The vectors $\tilde{f}(j)$, $\tilde{g}(j')$ are in one-to-one correspondence with $f(a_i^\dagger, j)$, $g(b_l^\dagger, j')$, however, they *forget* about the mode structure specified by $\{a_i\}$, $\{b_l\}$. Now arbitrary vector in $\mathcal{H}_A$ has a form $w = \sum_j w_j \tilde{f}(j)$, and a scalar product between arbitrary two vectors w and z reads:

$$\langle w | z \rangle_{\mathcal{H}_A} = \sum_j (w_j)^* z_j, \tag{11}$$

and analogous relations hold for vectors in $\mathcal{H}_B$. Note that, since the set of indices $\{j, j'\}$ is countable, the Hilbert spaces $\mathcal{H}_{A(B)}$ are, in fact, separable.

Now we define a linear map $\mathcal{I} : \mathcal{F}(\mathcal{H}_{\mathcal{AB}}) \to \mathcal{H}_{\mathcal{A}} \otimes \mathcal{H}_{\mathcal{B}}$ by specifying its action on basis elements of $\mathcal{F}(\mathcal{H}_{\mathcal{AB}})$:

$$\mathcal{I}(|j, j'\rangle) = \mathcal{I}\left(f\left(a_i^\dagger, j\right) g\left(b_l^\dagger, j'\right) |\Omega\rangle\right) := \tilde{f}(j) \otimes \tilde{g}(j'), \tag{12}$$

in which the tensor product in the definition refers to a standard algebraic tensor product between $\mathcal{H}_{\mathcal{A}}$ and $\mathcal{H}_{\mathcal{B}}$. The map $\mathcal{I}$ is clearly bijective. It also preserves scalar product:

$$\begin{aligned}\langle kk' | jj' \rangle = \delta_{k,j}\delta_{k',j'} &= \langle \Omega | g\left(b_l^\dagger, k'\right)^\dagger f\left(a_i^\dagger, k\right)^\dagger f\left(a_i^\dagger, j\right) g\left(b_l^\dagger, j'\right) |\Omega\rangle \\ &\xrightarrow{\mathcal{I}()} \langle \tilde{f}(k) \otimes \tilde{g}(k') | \tilde{f}(j) \otimes \tilde{g}(j') \rangle_{\mathcal{H}_{\mathcal{A}} \otimes \mathcal{H}_{\mathcal{B}}} \\ &= \langle \tilde{f}(k) | \tilde{f}(j) \rangle_{\mathcal{H}_A} \langle \tilde{g}(k') | \tilde{g}(j') \rangle_{\mathcal{H}_B} = \delta_{k,j}\delta_{k',j'}.\end{aligned} \tag{13}$$

Therefore, map $\mathcal{I}$ is an isomorphism, and $\mathcal{F}(\mathcal{H}_{\mathcal{AB}})$ and $\mathcal{H}_{\mathcal{A}} \otimes \mathcal{H}_{\mathcal{B}}$ are isomorphic. Note that this is not a *canonical* isomorphism, since it is basis-dependent, similarly to a Choi–Jamiolkowski isomorphism [28, 29].

Since by construction both $\mathcal{H}_{\mathcal{A}}$ and $\mathcal{H}_{\mathcal{B}}$ are separable Hilbert spaces, any vector $\phi \in \mathcal{H}_{\mathcal{A}} \otimes \mathcal{H}_{\mathcal{B}}$ possesses a Schmidt decomposition:

$$\phi = \sum_t \lambda_t \tilde{F}(t) \otimes \tilde{G}(t), \tag{14}$$

with $\tilde{F}(t)$, $\tilde{G}(t)$ being some orthonormal basis vectors in spaces $\mathcal{H}_{A(B)}$.

Now, let us consider an arbitrary state $|\psi\rangle$ in $\mathcal{F}(\mathcal{H}_{\mathcal{AB}})$ and find its Schmidt decomposition. By using isomorphism $\mathcal{I}$ one gets:

$$|\psi\rangle = \mathcal{I}^{-1}(\mathcal{I}(|\psi\rangle)) = \mathcal{I}^{-1}\left(\sum_t \lambda_t \tilde{F}(t) \otimes \tilde{G}(t)\right) = \sum_t \lambda_t \mathcal{I}^{-1}\left(\tilde{F}(t) \otimes \tilde{G}(t)\right), \tag{15}$$

in which we used Schmidt decomposition (14) for the vector $\mathcal{I}(|\psi\rangle)$. Since $\tilde{F}(t)$ and $\tilde{G}(t)$ are clearly linear combinations of original basis vectors $\tilde{F}(t) = \sum_j q_j^t \tilde{f}(j)$, $\tilde{G}(t) = \sum_{j'} p_{j'}^t \tilde{g}(j')$, we have:

$$\mathcal{I}^{-1}\left(\tilde{F}(t) \otimes \tilde{G}(t)\right) = \left[\sum_j q_j^t f\left(a_i^\dagger, j\right)\right] \left[\sum_{j'} p_{j'}^t g\left(b_l^\dagger, j'\right)\right] |\Omega\rangle = F\left(a_i^\dagger, t\right) G\left(b_l^\dagger, t\right) |\Omega\rangle, \tag{16}$$

where $F(a_i^\dagger, t)$, $G(b_l^\dagger, t)$ are polynomials of creation operators in corresponding groups of modes $\{a_i\}$, $\{b_l\}$.

Finally we obtain:

$$|\psi\rangle = \sum_t \lambda_t F\left(a_i^\dagger, t\right) G\left(b_l^\dagger, t\right) |\Omega\rangle. \tag{17}$$

As inverse isomorphism $\mathcal{I}^{-1}$ preserves orthogonality, all terms in (17) are orthogonal to each other and what is more locally orthogonal:

$$\langle \Omega | F\left(a_i^\dagger, t\right)^\dagger F\left(a_i^\dagger, t'\right) |\Omega\rangle = \langle \Omega | G\left(b_l^\dagger, t\right)^\dagger G\left(b_l^\dagger, t'\right) |\Omega\rangle = \delta_{t,t'}. \tag{18}$$

Furthermore, due to uniqueness of the Schmidt decomposition of states from $\mathcal{H}_\mathcal{A} \otimes \mathcal{H}_\mathcal{B}$, the decomposition on the Fock space is also unique for the given partition $\{a_i\}$, $\{b_l\}$. This uniqueness is up to the choice of the phase factor for polynomials $F(a_i^\dagger, t)$, $G(b_l^\dagger, t)$ which however always results in the same phase factor for the state $F(a_i^\dagger, t)G(b_l^\dagger, t)|\Omega\rangle$.This provides a generalization of the Schmidt decomposition for an arbitrary vector in a Fock space, built from a single-particle space with two separated groups of modes.

Note that, a crucial step in building this decomposition is the choice of mutually orthogonal groups of modes $\{a_i\}$, $\{b_l\}$, which allows for the construction of subsystems and associating separate Hilbert spaces to them. However, the choice of particular local bases within the modes $\{a_i\}$ and $\{b_l\}$ is irrelevant for Schmidt decomposition, as it is unique. The different choice of modes local to subsystems, respectively $\{a_i'\}$ and $\{b_l'\}$, results only in rewriting operators $F(a_i^\dagger, t)$, $G(b_l^\dagger, t)$ in terms of these modes and thus finding different polynomials of creation operators in these modes which satisfy $F'(a_i'\dagger, t) = F(a_i^\dagger, t)$ and $G'(b_l'\dagger, t) = G(b_l^\dagger, t)$.

4. Gisin's theorem for quantum fields

Let us now prove the central result of the work which states that for any pure entangled state there exists a Bell inequality which is violated. Let us alternatively state the notion of mode entanglement in terms of Schmidt decomposition, based on definition of separable states (7), what will become useful in further considerations. The following statement clearly is a consequence of the fact that the Schmidt decomposition (17) exists for any pure state of the field and is unique.

Lemma 1. *The state of the field $|\psi\rangle$ is separable with respect to the partition of modes into families $\{a_i\}$, $\{b_l\}$ iff its Schmidt decomposition (17) admits $\exists! \lambda_t \neq 0$, that is:*

$$|\psi\rangle = F\left(a_i^\dagger, 1\right) G\left(b_l^\dagger, 1\right) |\Omega\rangle, \tag{19}$$

and otherwise state $|\psi\rangle$ is entangled.

In other words, state is entangled iff its Schmidt decomposition has at least two non-zero terms, i.e. it has a form:

$$\begin{aligned} |\psi_{\text{ent}}\rangle &= \lambda_1 F\left(a_i^\dagger, 1\right) G\left(b_l^\dagger, 1\right) |\Omega\rangle + \lambda_2 F\left(a_i^\dagger, 2\right) G\left(b_l^\dagger, 2\right) |\Omega\rangle \lambda_R |R\rangle \\ &= \sqrt{|\lambda_1|^2 + |\lambda_2|^2} |\phi_{12}\rangle + \lambda_R |R\rangle, \end{aligned} \tag{20}$$

where $|R\rangle$ is some state emerging from the terms for $t > 2$ which is orthogonal to the first two terms and λ_R is the amplitude corresponding to this state (it can be zero). In the above representation of a Schmidt decomposition we have introduced a partition of the decomposed state into a 2×2 dimensional subspace corresponding to the two highest Schmidt coefficients (which in the case of entangled states are necessarily non-zero), and the rest. This partition is crucial in our proof, as the Bell inequality violation will be firstly shown on the effective two-qubit subspace related to λ_1 and λ_2.

Now, assume that the set $\mathcal{S} := \{F(a_i^\dagger, t)G(b_l^\dagger, t)|\Omega\rangle\}_t$ is complete (spans the entire Fock space $\mathcal{F}(\mathcal{H}_{\mathcal{AB}})$). This holds without loss of generality, as if the decomposition of the state $|\psi\rangle$ does not contain terms corresponding to the full complete set, one can extend the set $\mathcal{S}$ to a complete set by choosing an orthogonal basis of the Schmidt form in the orthogonal complement of this set. In such a case, the basis elements of the extended part of the set $\mathcal{S}$ are included in the Schmidt decomposition of a state $|\psi\rangle$ simply with $\lambda_t = 0$. Consider now a subspace of a space of all well-defined operators on the Fock space $\mathcal{F}(\mathcal{H}_{\mathcal{AB}})$ spanned by the following operators:

$$P_{ab}^{k,k',n,n'} = F\left(a_i^\dagger, k\right) G\left(b_l^\dagger, n\right) |\Omega\rangle\langle\Omega| G\left(b_l^\dagger, n'\right)^\dagger F\left(a_i^\dagger, k'\right)^\dagger, \tag{21}$$

where $k, k', n, n' \in \{1, 2\}$. Local operators which represent observables local with respect to the parties can be written as:

$$\begin{aligned} P_a^{k,k'} &= \sum_t F\left(a_i^\dagger, k\right) G\left(b_l^\dagger, t\right) |\Omega\rangle\langle\Omega| G\left(b_l^\dagger, t\right)^\dagger F\left(a_i^\dagger, k'\right)^\dagger, \\ P_b^{k,k'} &= \sum_t F\left(a_i^\dagger, t\right) G\left(b_l^\dagger, k\right) |\Omega\rangle\langle\Omega| G\left(b_l^\dagger, k'\right)^\dagger F\left(a_i^\dagger, t\right)^\dagger. \end{aligned} \tag{22}$$

Clearly expectation value of any operator $\hat{O}$ from the subspace spanned by operators (21) and (22) calculated on the state $|\psi_{\text{ent}}\rangle$ consists of two terms:

$$\langle \hat{O} \rangle_{\psi_{\text{ent}}} = \left(|\lambda_1|^2 + |\lambda_2|^2\right) \langle \hat{O} \rangle_{\phi_{12}} + |\lambda_R|^2 \langle \hat{O} \rangle_R = \left(|\lambda_1|^2 + |\lambda_2|^2\right) \langle \hat{O} \rangle_{\phi_{12}}, \tag{23}$$

where the second term in the first row is equal to zero as the state $|R\rangle\langle R|$ is in the subspace orthogonal to all operators (21).

Clearly $|\phi_{12}\rangle$ is entangled in the considered 2×2 dimensional subspace, and therefore from the original Gisin's theorem there exists a Clauser–Horne–Shimony–Holt (CHSH) inequality, which is violated by such a state on the positive side. Following [11] we can directly construct such a CHSH inequality and the corresponding observables and settings leading to a violation. The CHSH inequality from Gisin's original work has the following conditional form:

$$E\left(\vec{\alpha},\vec{\beta}\right)-E\left(\vec{\alpha},\vec{\beta}'\right)+E\left(\vec{\alpha}',\vec{\beta}\right)+E\left(\vec{\alpha}',\vec{\beta}'\right)\leqslant 2,\ \text{if}\ E\left(\vec{\alpha},\vec{\beta}\right)\geqslant E\left(\vec{\alpha},\vec{\beta}'\right),$$
$$E\left(\vec{\alpha},\vec{\beta}'\right)-E\left(\vec{\alpha},\vec{\beta}\right)+E\left(\vec{\alpha}',\vec{\beta}\right)+E\left(\vec{\alpha}',\vec{\beta}'\right)\leqslant 2,\ \text{if}\ E\left(\vec{\alpha},\vec{\beta}\right)< E\left(\vec{\alpha},\vec{\beta}'\right), \tag{24}$$

where the correlation function for two-qubit system is defined as $E(\vec{\alpha},\vec{\beta})=\langle\vec{\alpha}\cdot\vec{\sigma}\otimes\vec{\beta}\cdot\vec{\sigma}\rangle$. The settings are parametrized by vectors:

$$\begin{aligned}\vec{\alpha}&=(\sin\alpha,0,\cos\alpha),\\ \vec{\beta}&=(\sin\beta,0,\cos\beta),\\ \vec{\alpha}'&=(\sin\alpha',0,\cos\alpha'),\\ \vec{\beta}'&=(\sin\beta',0,\cos\beta').\end{aligned} \tag{25}$$

Assuming the two-qubit state in a specific Schmidt form:

$$|\psi\rangle=\lambda_1|01\rangle+\lambda_2|10\rangle, \tag{26}$$

the optimal settings are specified by the following angles:

$$\begin{aligned}\alpha&=0,\\ \alpha'&=-\operatorname{sign}(\lambda_1\lambda_2)\tfrac{\pi}{2},\\ \cos\beta=-\cos\beta'&=(1+4|\lambda_1\lambda_2|)^{-\frac{1}{2}}.\end{aligned} \tag{27}$$

In order to apply the CHSH inequality (24) to the state $|\phi_{12}\rangle$ one has to translate qubit observables:

$$\vec{\alpha}\cdot\vec{\sigma}\otimes\vec{\beta}\cdot\vec{\sigma}$$

to field operators spanned by the local to parties operators (22). Since the two effective qubit subspaces in $|\phi_{12}\rangle$ are spanned by operators $\{F(a_i^\dagger,1),F(a_i^\dagger,2)\}$ and respectively $\{G(b_l^\dagger,1),G(b_l^\dagger,2)\}$, the field operators representing qubit Pauli observables have the following form:

$$\begin{aligned}\Sigma_x(a_i)&=P_a^{12}+P_a^{21},\\ \Sigma_y(a_i)&=-i\left(P_a^{12}-P_a^{21}\right),\\ \Sigma_z(a_i)&=P_a^{11}-P_a^{22},\\ \Sigma_x(b_l)&=P_b^{12}+P_b^{21},\\ \Sigma_y(b_l)&=-i\left(P_b^{21}-P_b^{12}\right),\\ \Sigma_z(b_l)&=P_b^{22}-P_b^{11},\end{aligned} \tag{28}$$

where for the operators on modes $\{b_l\}$ a flip of basis elements is taken into account in accordance with (26) (namely for the second effective qubit $G(b_l^\dagger,1)$ plays the role of $|1\rangle$ and $G(b_l^\dagger,2)$ of $|0\rangle$). In the above formulae the operators $P_a^{kk'}$ and $P_b^{kk'}$ are counterparts of raising and lowering operators σ^+ and σ^- in the first quantization picture, and they are defined by equation (22). Finally, an arbitrary qubit observable is mapped into the following field observable:

$$\vec{\alpha}\cdot\vec{\sigma}\otimes\vec{\beta}\cdot\vec{\sigma}\mapsto\left(\vec{\alpha}\cdot\vec{\Sigma}(a_i)\right)\left(\vec{\beta}\cdot\vec{\Sigma}(b_l)\right), \tag{29}$$

in which $\vec{\Sigma}(a_i)=(\Sigma_x(a_i),\Sigma_y(a_i),\Sigma_z(a_i))$ and analogously for $\vec{\Sigma}(b_l)$. Finally, the CHSH inequality for fields is built using the following correlation function:

$$\mathcal{E}\left(\vec{\alpha},\vec{\beta}\right)_{\phi_{12}}=\left\langle\left(\vec{\alpha}\cdot\vec{\Sigma}(a_i)\right)\left(\vec{\beta}\cdot\vec{\Sigma}(b_l)\right)\right\rangle_{\phi_{12}}, \tag{30}$$

in which the caligraphic notation on the left-hand-side indicates that we deal with the correlation function for fields not for qubits. By construction, one of the following CHSH inequalities is always violated for the state $|\phi_{12}\rangle$:

$$\mathcal{E}\left(\vec{\alpha},\vec{\beta}\right)_{\phi_{12}} - \mathcal{E}\left(\vec{\alpha},\vec{\beta}'\right)_{\phi_{12}} + \mathcal{E}\left(\vec{\alpha}',\vec{\beta}\right)_{\phi_{12}} + \mathcal{E}\left(\vec{\alpha}',\vec{\beta}'\right)_{\phi_{12}} \leqslant 2, \text{ if } \mathcal{E}\left(\vec{\alpha},\vec{\beta}\right)_{\phi_{12}} \geqslant \mathcal{E}\left(\vec{\alpha},\vec{\beta}'\right)_{\phi_{12}},$$
$$\mathcal{E}\left(\vec{\alpha},\vec{\beta}'\right)_{\phi_{12}} - \mathcal{E}\left(\vec{\alpha},\vec{\beta}\right)_{\phi_{12}} + \mathcal{E}\left(\vec{\alpha}',\vec{\beta}\right)_{\phi_{12}} + \mathcal{E}\left(\vec{\alpha}',\vec{\beta}'\right)_{\phi_{12}} \leqslant 2, \text{ if } \mathcal{E}\left(\vec{\alpha},\vec{\beta}\right)_{\phi_{12}} < \mathcal{E}\left(\vec{\alpha},\vec{\beta}'\right)_{\phi_{12}}. \quad (31)$$

Due to the factor $(|\lambda_1|^2 + |\lambda_2|^2)$ in the formula (23), the above inequalities *need not be violated on the entire initial state* $|\psi_{ent}\rangle$. However, we can easily prove that the corresponding CH inequalities *are violated* on $|\psi_{ent}\rangle$ whenever the CHSH inequalities are violated solely on $|\phi_{12}\rangle$. Let us start from defining these new inequalities. In 2×2 dimensional spaces a positive violation of the CHSH inequality is equivalent to a positive violation of a CH inequality (see e.g. [30], section 2.5.2). The correspondence between the two inequalities is due to the following relation between correlation functions and probabilities:

$$E\left(\vec{\alpha},\vec{\beta}\right) = 4p\left(0,0|\vec{\alpha},\vec{\beta}\right) - 2p\left(0|\vec{\alpha}\right) - 2p\left(0|\vec{\beta}\right) + 1, \quad (32)$$

which holds whenever the outcomes of the measured observables are dichotomic. In the above we have chosen outcomes labeled by $(0,0)$, however, any choice of the outcomes is valid, what is important is that they are fixed in the above relation. In our scenario, the field observables (28) are dichotomic when restricted to the subspace spanned by the first two Schmidt bases elements in (20), therefore, on this subspace the mapping between CHSH and CH inequality holds exactly. The CH inequalities corresponding to the CHSH inequalities (31) have the following form:

$$p\left(0,0|\vec{\alpha},\vec{\beta}\right) + p\left(0,0|\vec{\alpha}',\vec{\beta}\right) + p\left(0,0|\vec{\alpha}',\vec{\beta}'\right) - p\left(0,0|\vec{\alpha},\vec{\beta}'\right) - p\left(0|\vec{\alpha}'\right) - p\left(0|\vec{\beta}\right) \leqslant 0,$$
$$p\left(0,0|\vec{\alpha},\vec{\beta}'\right) + p\left(0,0|\vec{\alpha}',\vec{\beta}\right) + p\left(0,0|\vec{\alpha}',\vec{\beta}'\right) - p\left(0,0|\vec{\alpha},\vec{\beta}\right) - p\left(0|\vec{\alpha}'\right) - p\left(0|\vec{\beta}'\right) \leqslant 0, \quad (33)$$

in which the probabilities are specified as follows:

$$p\left(0,0|\vec{\alpha},\vec{\beta}\right) = \left\langle \tfrac{1}{4}\left(\mathbb{1}_A + \vec{\alpha}\cdot\vec{\Sigma}(a_i)\right)\left(\mathbb{1}_B - \vec{\beta}\cdot\vec{\Sigma}(b_l)\right)\right\rangle_{\phi_{12}},$$
$$p\left(0|\vec{\alpha}\right) = \left\langle \tfrac{1}{2}\left(\mathbb{1}_A + \vec{\alpha}\cdot\vec{\Sigma}(a_i)\right)\right\rangle_{\phi_{12}},$$
$$p\left(0|\vec{\beta}\right) = \left\langle \tfrac{1}{2}\left(\mathbb{1}_B - \vec{\beta}\cdot\vec{\Sigma}(b_l)\right)\right\rangle_{\phi_{12}}. \quad (34)$$

In the above formulas $\mathbb{1}_{A/B}$ denotes the following operators which act as projectors onto the local subspace of interest and identity on the second subsystem:

$$\mathbb{1}_A = P_a^{1,1} + P_a^{2,2},$$
$$\mathbb{1}_B = P_b^{1,1} + P_b^{2,2}. \quad (35)$$

Now, violation of one of the CHSH inequalities (31) on $|\phi_{12}\rangle$ implies violation of the corresponding CH inequality from among (33) on $|\phi_{12}\rangle$. It suffices to show that the CH inequality is then also violated on the entire state $|\psi_{\text{ent}}\rangle$. Let us denote the Bell operator for a CH inequality as $\hat{CH}$. Then whenever any of the CH inequalities (33) is violated, we have for the corresponding Bell operator: $\langle\hat{CH}\rangle_{\phi_{12}} > 0$. This yields:

$$\langle\hat{CH}\rangle_{\psi_{\text{ent}}} = \left(|\lambda_1|^2 + |\lambda_2|^2\right)\langle\hat{CH}\rangle_{\phi_{12}} > 0, \quad (36)$$

an therefore violation of the CH inequality on the state $|\phi_{12}\rangle$ implies a violation of the inequality by the state $|\psi_{\text{ent}}\rangle$. This ends the proof.

Note that the violation of the CHSH inequalities on the state $|\phi_{12}\rangle$ (31) *does not imply* violation of these inequalities on the entire state $|\psi_{\text{ent}}\rangle$, therefore the transition to the CH inequality is necessary for the proof to hold. The two inequalities are *not equivalent* on the entire state space, since then the measurements defined by operators (28) are no longer dichotomic. One has to be very careful when trying to prove CHSH inequality violation on the entire state space based on its violation on the subspace, since this can lead to false conclusions on Bell non-classicality, see e.g. [31].

4.1. Two distinguishable fields

One can also consider the entanglement of two or any finite number of fields species. For simplicity, let us consider the case of two fields as the other cases follow analogously. In such a case, the state space is given by the tensor product of two Fock spaces $\mathcal{F}(\mathcal{H}_{AB})_q \otimes \mathcal{F}'(\mathcal{H}_{A'B'})_{q'}$ where we already assumed partition of modes into families $\{a_i\}$, $\{b_l\}$ and $\{a_i'\}$, $\{b_l'\}$. Note that one of those families of modes per primed or unprimed pair could be empty. Once again, one can represent the occupation number basis vectors for the first field as $\vec{n}^j, \vec{m}^{j'}$ and $(\vec{n'})^j, (\vec{m'})^{j'}$ for the second using suitable monomials of creation operators in modes corresponding to the considered partition:

$$|\vec{n}^j, (\vec{n'})^j; \vec{m}^{j'}, (\vec{m'})^{j'}\rangle = f\left(a_i^\dagger, (a_i')^\dagger, j\right) g\left(b_l^\dagger, (b_l')^\dagger, j'\right)|\Omega\rangle, \quad (37)$$

where indices j, j' are again countable and $|\Omega\rangle$ stands for tensor product of vacuum states of both fields. We use here the fact that creation operators for distinguishable fields commute, and therefore one can group them as it is presented on the right-hand side. Now one can see that the isomorphism (12) can be trivially generalized to this case. This results in the isomorphism between space $\mathcal{F}(\mathcal{H}_{AB})_q \otimes \mathcal{F}'(\mathcal{H}_{A'B'})_{q'}$ and separable space $\mathcal{H}_{A,A'} \otimes \mathcal{H}_{B,B'}$ where $\mathcal{H}_{A,A'(B,B')}$ are counterparts to $\mathcal{H}_{A,(B)}$. Once again, one can apply the Schmidt decomposition on the state mapped to $\mathcal{H}_{A,A'} \otimes \mathcal{H}_{B,B'}$ in order to obtain the decomposed state in the tensor product of Fock spaces. The resulting general form of the Schmidt decomposition of the state $|\psi\rangle \in \mathcal{F}(\mathcal{H}_{AB})_q \otimes \mathcal{F}'(\mathcal{H}_{A'B'})_{q'}$ is the following:

$$|\psi\rangle = \sum_t \lambda_t F\left(a_i^\dagger, (a_i')^\dagger, t\right) G\left(b_l^\dagger, (b_l')^\dagger, t\right)|\Omega\rangle, \quad (38)$$

where $F(a_i^\dagger, (a_i')^\dagger, t)$, $G(b_l^\dagger, (b_l')^\dagger, t)$ are polynomials of creation operators of respective modes. Upon this one can build a CH inequality for any entangled pure state, which would be violated in full analogy to the construction ending at formula (36).

5. Non-separable Hilbert spaces

The issue of whether non-separable Hilbert spaces are useful for Quantum Field Theory is subtle and controversial. On the one hand, a separable Hilbert space is sufficient to describe scattering processes (see, e.g. [32], chapter 2.6). On the other hand, for some applications, it is convenient to introduce *big* Hilbert space $\mathcal{H}' = \bigoplus_{n=0}^{\infty} \mathcal{H}^{\otimes n}$, where $\mathcal{H}^{\otimes n}$ for $n \to \infty$ is treated as an *infinite tensor product*, which describes the system of *actually infinite* number of particles. Such *big* Hilbert space is non-separable and contains as its subspaces all Fock spaces emerging from all different choices of basis solutions for field equations (these Fock spaces are defined in a similar way, but with $\mathcal{H}^{\otimes n}$ interpreted as representing only *potentially infinite* number of particles). This *big* Hilbert space $\mathcal{H}'$ is, in fact, built from these Fock spaces. The creation and annihilation operators corresponding to these Fock spaces are then related by non-unitary transformations (for example, by Bogoliubov transformations) leading to appearance of an effective description in terms of quasi-particles [33]. Then the infinite particle states are effectively hidden in different 'vacuum' states of the corresponding Fock spaces. *Big* non-separable Hilbert space is useful, for example, in statistical mechanics for description of phase transitions: taking the thermodynamic limit, in which the density of a system remains constant, while its spatial dimensions tend to infinity, demands considering actually infinite number of particles in the system.

Therefore, in principle, one can consider the *big* multimode Hilbert space $\mathcal{H}'$, with modes grouped into two disjoint subsets $\mathcal{A}$ and $\mathcal{B}$, which define the local structure for a Bell-type reasoning. This space is formally spanned by number states $\{|\vec{n}_\nu\rangle_{\mathcal{A}}|\vec{m}_\mu\rangle_{\mathcal{B}}\}$, in which vectors $\vec{n}_\nu$ and $\vec{m}_\mu$ represent infinite sequences of integers without cut-off conditions used in defining the Fock space. Such sets of vectors are certainly uncountable. Note that the cardinality of this set of basis vectors is $\aleph_0^{\aleph_0}$ which is the same as saying that its cardinality is of the continuum $\mathfrak{c}$ and therefore it can be indexed symbolically by real indices ν, μ. In order to justify in what sense Gisin's theorem generalizes to such a case, we have to recall a very important result in mathematical physics, namely the generalization of Gleason's theorem for non-separable Hilbert spaces. Recall that in the case of separable Hilbert spaces, Gleason's theorem states that any assignment $m : \{\hat{\Pi}_i\} \mapsto [0,1]$ of a probability distribution to a family of projectors onto closed subspaces of a Hilbert space of dimension greater than two is represented by $m(\hat{\Pi}_i) = \mathrm{Tr}(\rho_m \hat{\Pi}_i)$, in which ρ_m is a normalized positive-semidefinite matrix, typically called a density matrix. This theorem has been generalized to the case of a non-separable Hilbert space [34]. This generalization states that if the cardinality of a set of basis vectors in a given Hilbert space is given by the Ulam number and under the assumption of the continuum hypothesis, any assignment of a probability distribution $m : \{\hat{\Pi}_\eta\} \mapsto [0,1]$ to a (possibly uncountable) family of projectors onto closed subspaces of the Hilbert space is represented by $m(\hat{\Pi}_\eta) = \mathrm{Tr}(\rho_m \hat{\Pi}_{\mathcal{K}_m} \hat{\Pi}_\eta)$, in which $\hat{\Pi}_{\mathcal{K}_m}$ is a projector onto a separable subspace $\mathcal{K}_m$ of the entire Hilbert space and ρ_m is a state on the separable space $\mathcal{K}_m$. Therefore, one can say that any state on a non-separable Hilbert space is in fact represented by a state on a separable subspace. In the context of the *big* Hilbert space introduced in the previous paragraph, as the continuum $\mathfrak{c}$ is an Ulam number, this theorem implies that any state on the *big* space is represented by a state belonging to some Fock space or at most finite combinations of them. Since our generalization of Gisin's theorem works for any state on any Fock space, it effectively works for any state defined on the *big* Hilbert space. In appendix the Schmidt decomposition of the state in $\mathcal{H}'$ in terms of extended occupation number basis is presented, which then allows for analogous direct construction of a CH inequality that is always violated for an entangled state of the field modes.

6. Examples

Let us consider a few examples of Schmidt decompositions of entangled states with undefined particle numbers. The first example is of particular importance, as for this state, one cannot reveal its entanglement by projecting it into specific particle numbers and trying to map the problem to the language of first quantization. Therefore, this example in particular was not covered by previous generalizations of Gisin's theorem. This example is the two-mode squeezed vacuum state, which in its Schmidt form can be written as:

$$|\Psi\rangle = \sum_{n=0}^{\infty} \lambda_{n+1} \left(\hat{a}_1^\dagger\right)^n \left(\hat{b}_1^\dagger\right)^n |\Omega\rangle = \sum_{n=0}^{\infty} \lambda_{n+1} |n;n\rangle. \tag{39}$$

Note that, here for clarity we use the following notation for Fock states:

$$|n_1, n_2, \ldots; m_1, m_2, \ldots\rangle := \frac{1}{\mathcal{N}_a \mathcal{N}_b} \left[\left(\hat{a}_1^\dagger\right)^{n_1} \left(\hat{a}_2^\dagger\right)^{n_2} \ldots\right] \left[\left(\hat{b}_1^\dagger\right)^{m_1} \left(\hat{b}_2^\dagger\right)^{m_2} \ldots\right] |\Omega\rangle, \tag{40}$$

with semicolon dividing again modes of the two subsystems. Now one can choose the following partition for investigating the CH inequality violation:

$$|\Psi\rangle = N_{\lambda_1\lambda_2} \left[\frac{1}{\sqrt{|\lambda_1|^2 + |\lambda_2|^2}} \left(\lambda_0 |0;0\rangle + \lambda_1 |1;1\rangle\right)\right] + \lambda_R |R\rangle, \tag{41}$$

in which $N_{\lambda_1\lambda_2} = \sqrt{|\lambda_1|^2 + |\lambda_2|^2}$. Here, the construction of the CH operator based on the operators (28) requires the ability to implement measurements that perform projections onto states of the form $\cos\theta|0\rangle + e^{i\phi}\sin\theta|1\rangle$. However, it is not known how to perform such a projection experimentally. One can find a violation of some Bell inequality for states from subspace in which the CH operator is constructed using homodyne measurements [35]. However, such measurements cannot project the state $|\Psi\rangle$ onto this subspace. Thus, testing CH inequalities based on Schmidt decomposition is not always feasible experimentally, and this problem is described in more detail in the next section. Still, this is only a technical limitation, and fundamentally, this state does not admit any LHV model.

However, there exist states with an undefined photon number for which one can experimentally test the CH inequality violation constructed as in (36). As an example we consider the 2×2 bright squeezed vacuum state of four modes $\{a_1, a_2\}$, $\{b_1, b_2\}$ [4], which can be put into the following Schmidt form :

$$|\psi_-\rangle = \frac{1}{\cosh^2(\Gamma)} \sum_{n=0}^{\infty} \tanh^n(\Gamma) \sum_{m=0}^{n} (-1)^m |(n-m), m; m, (n-m)\rangle, \tag{42}$$

where the parameter Γ denotes the amplification gain. Consider the following partition of the state:

$$|\psi_-\rangle = \frac{\sqrt{2}\tanh(\Gamma)}{\cosh^2(\Gamma)} \left[\frac{1}{\sqrt{2}} \left(|1,0;0,1\rangle - |0,1;1,0\rangle\right)\right] + \alpha_R |R\rangle. \tag{43}$$

If the modes would represent a possible photon paths (two per subsystem) then the first term is simply a typical dual-rail-encoded singlet. The measurements corresponding to the operator subspace (22) are simply given by Stokes operators or Sign Stokes operators [36, 37] restricted to the single-particle subspace and act on it like Pauli operators. Such operators can be implemented using photon-number-resolving detectors. However, taking another partition of the state (42) including states with more than one photon, one would need to, for example, implement generalized Pauli operators for quantum fields [38], the experimental realization of which is unclear.

As a final example we consider the BGHZ state [39] of six modes $\{a_1,a_2,a_3,a_4\}$, $\{b_1,b_2\}$ which is a generalization of the GHZ state to states with an undefined number of photons. This state emerges from a generalization of two-mode squeezing to three-mode squeezing. This state has the following Schmidt form for the chosen partition of modes:

$$\begin{aligned}|BGHZ\rangle &= \sum_{k=0}^{\infty}\sum_{m=0}^{k} C_{k-m}(\Gamma)\,C_m(\Gamma)\left(\hat{a}_1^\dagger\hat{a}_2^\dagger\hat{b}_1^\dagger\right)^{k-m}\left(\hat{a}_3^\dagger\hat{a}_4^\dagger\hat{b}_2^\dagger\right)^{m}|\Omega\rangle \\ &= \sum_{k=0}^{\infty}\sum_{m=0}^{k} C_{k-m}(\Gamma)\,C_m(\Gamma)\,|k-m,k-m,m,m;k-m,m\rangle,\end{aligned} \tag{44}$$

where $C_q(\Gamma)$ are coefficients dependent on amplification gain Γ. Now we can choose the relevant terms in the Schmidt decomposition for the construction of the CH inequality as follows:

$$|BGHZ\rangle = \alpha_{12}\left[\frac{1}{\sqrt{2}}\left(|1,1,0,0;1,0\rangle + |0,0,1,1;0,1\rangle\right)\right] + \alpha_R|R\rangle. \tag{45}$$

The first term is simply a polarization or path entangled GHZ state with two of typical three subsystems $\{a_1,a_3\}$, $\{a_2,a_4\}$, $\{b_1,b_2\}$ merged into one. However, the projectors necessary for the violation of the CH inequality (33) do not have a known experimental realization as it requires performing Bell-state measurement within passive linear optics. However, if one considers the BGHZ state after single-photon subtraction among modes a_2,a_4 one gets:

$$|BGHZ\rangle_s = \alpha'_{12}\left[\frac{1}{\sqrt{2}}\left(|1,0,0,0;1,0\rangle + |0,0,1,0;0,1\rangle\right)\right] + \alpha'_R|R\rangle. \tag{46}$$

Due to this modification the suitable measurements for CH inequality violation have their experimental realization again as Stokes operators restricted to the single-photon subspace.

One can see that while the construction of the CH inequality (33) is purely abstract, in some circumstances its violation could be, in principle, measured using current technology.

7. Sufficient condition for the necessity of applying non-projective POVMs or other tricks

As noted in the previous section, there are many entangled states of quantum fields for which projective measurements are not sufficient to reveal their non-classical behavior. The reason for that is the impossibility of experimental realization of projections onto the states which are superpositions of states with different numbers of particles in the same mode like $(|0\rangle + |1\rangle)/\sqrt{2}$. Therefore, some non-projective measurements are necessary in such circumstances. In particular in quantum optics those are realized through addition of ancillary modes with coherent states to perform homodyne measurements. One can also, at least in some cases, engineer the ancillary state for the examined state in such a way that the violation can converge to the ideal case [40] (however, it is not known if the preparation of such ancillas is experimentally feasible). The Schmidt decomposition allows us to determine if such measurements are necessary. We formulate the following theorem:

Theorem 1. *The sufficient condition for the necessity of using ancillary resources (such as coherent states in ancillary modes or postselection) for experimental revealing of non-classicality of entangled state $|\psi\rangle$ can be formulated as follows: all projections of the state $|\psi\rangle$ into the subspace given by $\sum_i n_i = n$, $\sum_{i'} m_{i'} = m$ have Schmidt rank 1 i.e.*

$$\forall_{n,m}\frac{1}{N}\Pi_{nm}|\psi\rangle = F^n\left(a_i^\dagger,1\right)G^m\left(b_l^\dagger,1\right)|\Omega\rangle, \tag{47}$$

where N is a normalization factor, Π_{nm} is a projector onto the subspace considered, and $F^n(a_i^\dagger,1)$, $G^m(b_l^\dagger,1)$ are polynomials of creation operators of the order n, m respectively.

Note that one can write projector $\hat{\Pi}_{n,m}$ as follows:

$$\hat{\Pi}_{n,m} = \sum_{j|\sum n_i^j = n}\ \sum_{j'|\sum m_i^{j'} = m} |\vec{n}^j,\vec{m}^{j'}\rangle\langle\vec{n}^j,\vec{m}^{j'}|. \tag{48}$$

This Theorem is followed by the corollary:

Corollary 1. *The necessary condition for revealing non-classicality of an entangled state $|\psi\rangle$ with experimentally realizable projective measurements can be formulated as follows: There exists a projection of the state $|\psi\rangle$ into the subspace given by $\sum_i n_i = n, \sum_{i'} m_{i'} = m$ which have Schmidt rank higher than 1 i.e.*

$$\exists_{n,m}\exists_{\alpha_i,\alpha_j\neq 0}\frac{1}{N}\Pi_{nm}|\psi\rangle = \sum_t \alpha_t F^n\left(a_i^\dagger, t\right) G^m\left(b_l^\dagger, t\right)|\Omega\rangle. \tag{49}$$

The intuitive meaning of the above two statements is the following: whenever an *entangled* state of the optical field contains (mode) entanglement between terms with the same total photon number within the two subspaces corresponding to the two families of modes $\{a_i\}$ and $\{b_l\}$, then one can detect the non-classicality of the state with projectors realizable with passive linear optics. However, if there is no entanglement of this kind present in the state, one needs to utilize additional resources like ancillary modes or postselection in order to detect non-classicality of the state.

Let us give the proof of the theorem; the proof for the corollary follows immediately. Any projective measurement $\hat{M}$ that does not project into the superposition of states with different photon numbers always acts separately on the subspaces determined by the projectors Π_{nm}. Therefore, one can write:

$$\langle\hat{M}\rangle_\psi = \sum_{n,m}\langle\psi|\Pi_{nm}|\psi\rangle\langle\psi_{nm}|\hat{M}|\psi_{nm}\rangle, \tag{50}$$

where :

$$|\psi_{nm}\rangle = \frac{\Pi_{nm}|\psi\rangle}{\sqrt{\langle\psi|\Pi_{nm}|\psi\rangle}}. \tag{51}$$

Let $\hat{M}$ be the Bell operator, and let the state $|\psi\rangle$ fulfill the condition (47). This indicates that all $|\psi_{nm}\rangle$ are separable. Then the expectation value of the Bell operator is effectively taken over a separable state:

$$\hat{\rho}_{\text{sep}} = \sum_{nm}\langle\psi|\Pi_{nm}|\psi\rangle|\psi_{nm}\rangle\langle\psi_{nm}|. \tag{52}$$

Therefore, the expectation value of the Bell operator cannot violate the Bell inequality. Similarly, any entanglement or steering criterion based on projective measurement considered will not reveal non-classical behavior. This ends the proof.

The corollary 1 provides only necessary condition because while the class of observables which does not mix different photon number states is clearly at least partially realized in experiments, one does not know if all such operators can be experimentally implemented. Therefore, even if this condition is fulfilled, using ancillary modes might be necessary due to experimental but not fundamental reasons.

7.1. Introducing ancillary modes

When introducing ancillary modes (the state of which is separable with respect to the original one), the Schmidt form is modified only by multiplication of all terms by a single polynomial of creation operators per party. Let us denote by $A(c_k^\dagger)$, $B(d_h^\dagger)$ the polynomials that describe the state of the ancillary modes c_k, d_h for the party A and B respectively. Because states of ancillary modes are separable with respect to the state of modes a_i, b_l we can write the total state as follows:

$$\begin{aligned}|\Psi\rangle &= A\left(c_k^\dagger\right)|0\rangle B\left(d_h^\dagger\right)|0\rangle|\psi\rangle\\ &= \sum_t \lambda_t A\left(c_k^\dagger\right) F\left(a_i^\dagger, t\right) G\left(b_l^\dagger, t\right) B\left(d_h^\dagger\right)|\Omega\rangle\\ &= \sum_t \lambda_t F'\left(a_i^\dagger, c_k^\dagger, t\right) G'\left(b_l^\dagger, d_h^\dagger, t\right)|\Omega\rangle.\end{aligned} \tag{53}$$

Clearly the states generated by polynomials $F'(a_i^\dagger, c_k^\dagger, t)$, $G'(b_l^\dagger, d_h^\dagger, t)$ for all t are locally orthogonal. Therefore, equation (53) gives Schmidt form for total state with ancillary modes.

As an example, let us consider the state of a single-photon beamsplitted by a symmetric beamsplitter with output modes a_1, b_1 which is maximally entangled in the photon number basis:

$$|\phi\rangle = \frac{1}{\sqrt{2}}\left(\hat{a}_1^\dagger + \hat{b}_1^\dagger\right)|\Omega\rangle = \frac{1}{\sqrt{2}}\left(|0;1\rangle + |1;0\rangle\right). \tag{54}$$

Clearly, this state fulfills the condition (47) and therefore the entanglement of this state cannot be reached with straightforward photon number non-mixing projective measurements. Let us introduce two ancillary modes a_2, b_2 (one per party) occupied by coherent states with the same amplitude z resulting in the state in its Schmidt form:

$$|z\rangle_{a_2}|\phi\rangle|z\rangle_{b_2} = \frac{1}{\sqrt{2}}|z\rangle_{a_2}\hat{a}_1^\dagger|0;0\rangle|z\rangle_{b_2} + \frac{1}{\sqrt{2}}|z\rangle_{a_2}\hat{b}_1^\dagger|0;0\rangle|z\rangle_{b_2}. \tag{55}$$

Now consider the projection of this state into the subspace given by Π_{11}:

$$\Pi_{11}|z\rangle_{a_2}|\phi\rangle|z\rangle_{b_2} = \frac{e^{-|z|^2}\alpha}{\sqrt{2}}\left(\hat{a}_1^\dagger\hat{b}_2^\dagger + \hat{a}_2^\dagger\hat{b}_1^\dagger\right)|\Omega\rangle, \tag{56}$$

where

$$\Pi_{11} = |10;10\rangle\langle 10;10| + |01;10\rangle\langle 01;10| + |01;01\rangle\langle 01;01| + |10;01\rangle\langle 10;01|. \tag{57}$$

This projection has Schmidt rank 2 as, in fact, it is (after the normalization) a double-rail-encoded path-entangled Bell state. Therefore, after adding ancillary modes, condition (47) is no longer fulfilled and there is a possibility that one can reveal Bell non-classicality of this state using photon number non-mixing projective measurements. This is in fact the case, e.g. see [35, 41–43], where a CH inequality violation is observed for observables totally unrelated to Schmidt decomposition of the state (55). Let us, however, consider another strategy based on measuring the projected state (56). One can build upon its Schmidt decomposition the CH inequality of the form (33), which will be maximally 'violated' if one performs post-selection of results to events with a single photon per side resulting in the CH expression value $(\sqrt{2}-1)/2$ for any z. Note that if the projected state after normalization would be the full state, then one gets a real violation, as one does not have to use post-selection. Measurement which leads to such result could be realized using as observables combinations of Stokes operators projected to single-photon subspace as discussed in the example (43). However, applying the corresponding CH operator to the full state (55) without using post-selection will result in a lack of violation. This depicts that while one can reveal non-classicality (entanglement) of the state by post-selection to a specific number of particles shared between parties, the same criterion does not have to lead to a proper direct violation of local realism by the actual physical state (post-selection loophole). This additionally shows that generalizations of Gisin's theorem for fixed particle numbers were not sufficient to show that any entangled pure state does not admit LHV model.

7.2. Violation from projections into specific particle number

One could also ask for which states the CH inequality constructed for some projected state into a specific number of particles will be always violated by the total state. To answer this question let us note that the lack of violation of the CH inequality for the total state described above comes from modification of local probabilities of measuring an outcome specified in the CH inequality. More precisely, one can partition the CH operator constructed on the projected state into non-local (bipartite) and two local terms: $\hat{CH} = \hat{CH}_{\text{nl}} - \hat{CH}^a_{\text{loc}} - \hat{CH}^b_{\text{loc}}$ (see equations (33) and (34)). Then the expectation value of the CH operator evaluated on the full state is the following:

$$\langle\hat{CH}\rangle_\psi = \langle\hat{\Pi}_{nm}\rangle_\psi\langle\hat{CH}\rangle_{\psi_{n,m}} - \langle\hat{\Pi}_{n,m'\neq m}\rangle_\psi\langle\hat{CH}^a_{\text{loc}}\rangle_{\psi_{n,m}} - \langle\hat{\Pi}_{n'\neq n,m}\rangle_\psi\langle\hat{CH}^b_{\text{loc}}\rangle_{\psi_{n,m}}, \tag{58}$$

where $\hat{\Pi}_{q,k'\neq k}$ stands for a projector with number of particles different than k in the set of modes $\{b_l\}$ and q particles in the set of modes $\{a_i\}$ and analogously $\hat{\Pi}_{k'\neq k,q}$ for the set of modes reversed. Here, we used the fact that $\langle CH^{a(b)}_{\text{loc}}\rangle_{\psi_{n,m}} = \langle CH^{a(b)}_{\text{loc}}\rangle_{\psi_{n,m\neq m'}(\psi_{n\neq n',m})}$. Note that the last two terms are always negative whenever $\langle\hat{\Pi}_{n'\neq n,m}\rangle_\psi$ and $\langle\hat{\Pi}_{n,m'\neq m}\rangle_\psi$ are non-zero resulting in lowering the violation of the inequality and can even lead to not observing it. Therefore, the necessary and sufficient condition for violation of the considered type of CH inequality by the full state is:

$$\exists_{\Pi_{nm}}: \ r_{\psi_{n,m}} > 1 \wedge \langle\hat{\Pi}_{n,m'\neq m}\rangle_\psi\langle\hat{CH}^a_{\text{loc}}\rangle_{\psi_{n,m}} + \langle\hat{\Pi}_{n'\neq n,m}\rangle_\psi\langle\hat{CH}^b_{\text{loc}}\rangle_{\psi_{n,m}} < \langle\hat{\Pi}_{nm}\rangle_\psi\langle\hat{CH}\rangle_{\psi_{n,m}}, \tag{59}$$

where $r_{\psi_{n,m}}$ stands for Schmidt rank of state $|\psi_{nm}\rangle$. One can also find a simpler *sufficient* condition:

$$\exists_{\Pi_{nm}}: \ r_{\psi_{n,m}} > 1 \wedge \langle\hat{\Pi}_{n'\neq n,m}\rangle_\psi = \langle\hat{\Pi}_{n,m'\neq m}\rangle_\psi = 0, \tag{60}$$

which implies that the state $|\psi\rangle$ has the following easy to identify Schmidt form:

$$|\psi\rangle = \sum_t \alpha_t F^n\left(a_i^\dagger, t\right) G^m\left(b_l^\dagger, t\right)|\Omega\rangle + \sum_{t'} \alpha'_{t'} F'\left(a_i^\dagger, t'\right) G'\left(b_l^\dagger, t'\right)|\Omega\rangle, \tag{61}$$

where $F'(a_i^\dagger, t')$, $G'(b_l^\dagger, t')$ are polynomials of the corresponding creation operators such that:

$$\langle\Omega|F'\left(a_i^\dagger, t'\right)^\dagger G'\left(b_l^\dagger, t'\right)^\dagger \hat{\Pi}_{nm} F'\left(a_i^\dagger, t'\right) G'\left(b_l^\dagger, t'\right)|\Omega\rangle = 0. \tag{62}$$

Such a form, in fact, occurred in the examples of BGHZ (44) and BSV (42) states (for those states $\forall_{t'}\ \alpha'_{t'} = 0$).

8. Concluding remarks

In summary, in this work, we have proved that any pure mode-entangled state of quantum fields leads to a violation of some Bell inequality and, therefore, we provide a generalization of Gisin's theorem to quantum fields. This result also generalizes to non-separable Hilbert spaces used in the thermodynamic limits of quantum field theory. What is more, we provided a sufficient condition for the experimental need of introduction of ancillary resources out of a passive linear optics paradigm in order to measure Bell inequality violation. Finally, we have discussed several examples among which of particular importance are two-mode squeezed vacuum and beamsplitted single photon as entanglement of those states is distributed over states with different particle numbers (any of the cuts for specific particle number is not entangled); thus those are not covered by previous iterations of generalizations of Gisin's theorem.

Let us make a remark about the fundamental consequences of these results. This generalization of Gisin's theorem shows that quantum field theory predicts that any quantum measurement understood in the sense of standard quantum measurement theory [44–46] cannot be associated with the appearance of some LHV (local definite record of the outcome). This is because unitary evolution of the full system will lead to entanglement of the measured subsystem with the environment (measurement apparatus) trading for it inside coherences of the subsystem. However, as long as the entanglement is present, the LHV cannot appear.

Still, while the presented result provides the most general form of Gisin's theorem in the currently established theoretical quantum model of nature (quantum field theory), this does not give the final answer to the question if any entanglement remains in contradiction with local realism and thus also if mentioned predictions about measurement are generally valid. This is because we still do not have a unified quantum theory involving gravity, and the consequences of such construction do not have to lead to exactly the same predictions in general. One reason for that is the need to include in the description of the system degrees of freedom associated with the gravity which could have a different character than the quantum one [47] potentially making the global pure state description invalid.

In recent years, one observes an increasing interest in the analysis of entanglement of quantum fields in curved spacetimes [48–50] in pursuit of finding the nature of gravity, and also in multiple relativistic scenarios [51–53] that pose related mathematical problems. One of the main difficulties in such cases is the appearance of inequivalent representations of Fock spaces for different observers, which results in a lack of unambiguous description of particles, making the problem of entanglement much more subtle. Therefore, the problem of fully describing entanglement and its fundamental properties in such scenarios still poses an interesting and important problem. Our approach presented in this article can be applied in curved spacetimes as long as one has a unique Fock space in which all field modes under consideration can be described. This is the case of globally hyperbolic static space-times [54]. In the case of appearance of inequivalent Fock spaces for different observers the question of whether Gisin's theorem still holds does not have an answer, and even construction of a general scenario in order to meaningfully ask the question on relation between entanglement and Bell non-classicality is a challenging issue in itself and needs further investigation.

The another interesting problem to consider is whether in a similar manner one could generalize the results on multiparty Gisin's theorem, using for example techniques from [15].

Data availability statement

No new data were created or analyzed in this study.

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Appendix. Schmidt decomposition in non-separable Hilbert space

One can build the Schmidt decomposition of a state in a non-separable Hilbert space $\mathcal{H}'$ directly from the non-countable extended occupation number basis $|\vec{n}^j;\vec{m}^{j'}\rangle$ without restrictions $\sum_{i=1}^{\{a_i\}} n_i^j < \infty$, $\sum_{l=1}^{\{b_l\}} m_l^{j'} < \infty$. Let us recall that any state to which one can properly assign probabilities of outcomes has a non-zero distribution of probability only in the separable subspace $\mathcal{K}_\psi$ of $\mathcal{H}'$ and is equivalent to a state $|\psi\rangle$ from this subspace. One can build a countable basis $|k,k'\rangle$ in the subspace $\mathcal{K}_\psi$ using the basis vectors $|\vec{n}^j;\vec{m}^{j'}\rangle$ of $\mathcal{H}'$ as:

$$|k,k'\rangle = \int dj\,\beta_k(j)\int dj'\gamma_{k'}(j')\,|\vec{n}^j;\vec{m}^{j'}\rangle, \tag{A1}$$

where now j, j' are continuous indices, and $\beta_k(j), \gamma_{k'}(j')$ are amplitudes given by generalized functions. Note that these integrals could be, in some circumstances, reduced to sums over countable indices when amplitudes are given by countable sums of Dirac deltas. Then again one builds two abstract separable Hilbert spaces $\mathcal{H}_{A(B)}$ with one basis vector $\tilde{\beta}_k\,(\tilde{\gamma}_k')$ for each generalized function $\beta_k(j), \gamma_{k'}(j')$. Upon this, one builds the isomorphism $\mathcal{K}_\psi \to \mathcal{H}_A\otimes\mathcal{H}_B$ as $|k,k'\rangle \to \tilde{\beta}_k\otimes\tilde{\gamma}_k'$. Then one can again perform decomposition of $|\psi\rangle$ in $\mathcal{H}_A\otimes\mathcal{H}_B$ and transform it back to $\mathcal{K}_\psi$ reaching the decomposition of the form:

$$|\psi\rangle = \sum_t \alpha_t \sum_k \xi_k^t \sum_{k'} \zeta_{k'}^t |k,k'\rangle = \sum_t \alpha_t \left[\int dj \left(\sum_k \xi_k^t \beta_k\right)\int dj'\left(\sum_{k'}\zeta_{k'}^t\gamma_{k'}(j')\right)|\vec{n}^j;\vec{m}^{j'}\rangle\right]. \tag{A2}$$

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PAPER

Open dynamics of entanglement in mesoscopic bosonic systems

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Abstract

A key issue in quantum information is finding an adequate description of mesoscopic systems that is simpler than full quantum formalism yet retains crucial information about non-classical phenomena like entanglement. In particular, the study of fully bosonic systems undergoing open evolution is of great importance for the advancement of photonic quantum computing and communication. In this paper, we propose a mesoscopic description of such systems based on boson number correlations. This description allows for tracking Markovian open evolution of entanglement of both non-Gaussian and Gaussian states and their sub-Poissonian statistics. It can be viewed as a generalization of the reduced state of the field formalism (Alicki 2019 *Entropy* **21** 705), which by itself does not contain information about entanglement. As our approach adopts the structure of the description of two particles in terms of first quantization, it allows for broad intuitive usage of known tools. Using the proposed formalism, we show the robustness of entanglement against low-temperature damping for four-mode bright squeezed vacuum state and beam-splitted single photon. We also present a generalization of the Mandel Q parameter. Building upon this, we show that the entanglement of the state obtained by beam splitting of a single occupied mode is inherited from sub-Poissonian statistics of the input state.

1. Introduction

One of the important problems that is still developing in physics is the description of systems on the mesoscopic scale. This problem arises because full quantum treatment of large systems is not feasible. Classical description allows for an accurate depiction of the macroscopic systems; however, one can be interested in systems on the scale on which a full quantum description is not feasible, but with physical phenomena based on quantum features. In such a case, the classical paradigm becomes insufficient, and some intermediate methods are needed for this mesoscopic scale. The need to develop such theoretical tools emerges even more as experiments on this scale become nowadays feasible [1, 2]. This need is also fundamental from the perspective of quantum information, since its protocols require complicated quantum systems, and in their principles, they are based on quantum phenomena, such as superposition and entanglement [3].

Different semi-classical methods were introduced for the simplification of the problems, for example, the widely used parametric approximation [4, 5]. However, such techniques still require the full quantum description of some parts of the system. A different approach is to track observables that describe collective behavior of the system, e.g. total spin. Such a mean-field approach captures well macroscopic behavior of the system; however, information about quantum features is suppressed quickly with the number of particles. One can consider another collective observable, namely fluctuations instead of average values, as it is the case for the fluctuation algebra approach to mesoscopic systems [6, 7]. This technique is adopted in particular to describe entanglement in mesoscopic systems [8–10], and also different phenomena [11, 12]. Other methods were also used to describe the entanglement in mesoscopic systems [13–15].

One of the specific classes of systems for which mesoscopic descriptions are of great use is fully bosonic systems. The reason for this is that information encoded in bosonic modes is one of the promising avenues for implementing quantum information protocols. This is because, for example, information encoded in photons can be quickly transferred over long distances [16]. However, such systems are also affected by the decoherence effects coming from the environment, and their strict theoretical considerations require dealing with the whole infinite-dimensional Fock space, which can be unfeasible in multi-mode systems. The widely used method that simplifies the description is to track the evolution of the covariance matrix of position and momenta. This reduces the problem to finite-dimensional when a finite number of modes are considered [17–19]. In fact, this approach provides a full description of Gaussian states, and for non-Gaussian states, it can serve as a mesoscopic description. However, non-Gaussian features can be lost in this description, which can result in loss of useful information about quantum features of the state such as entanglement [20]. Another mesoscopic approach for bosonic systems that was recently proposed is the reduced state of the field (RSF) [21]. This formalism extends the mean-field approach with additional structure by the reduction of the state on the Fock space into the operator on the first quantization single-particle-like Hilbert space. This description was already applied for the analysis of the coronal heating phenomenon [22] and the dynamical Casimir effect [23]. However, it was shown that the RSF approach has some highly classical features and lacks information on quantum features interesting from the standpoint of quantum information. In particular, RSF does not store any information about distillable entanglement [24]. Moreover, for two mode Gaussian states, it was shown that it does not contain any information about entanglement.

In this paper, we identify degrees of freedom of bosonic systems that can be used in a mesoscopic description containing information about entanglement of both Gaussian and non-Gaussian states. Upon this, we propose an extended version of the RSF approach, which allows tracking the Markovian evolution of entanglement of bosonic fields. This is achieved by construction of a two-particle-like Hilbert space on which multi-mode bosonic state is mapped into the two-qudit state. Entanglement of this state is sufficient for the entanglement of the full state. In this approach, structures of typical finite-dimensional quantum systems emerge, and therefore one is left with a toolbox which is intuitive and based on well-known tools from quantum mechanics. This approach allowed us to show that the entanglement of the 2×2 bright squeezed vacuum state and the entangled two-mode single-photon state is robust against low-temperature damping by the environment. Our approach also allows for tracking particle number variance (fluctuations) and thus for tracking the non-classical phenomenon of sub-Poissonian statistics. In this context, we propose a generalization of the Mandel Q parameter, which can be calculated using the extended RSF. Upon this, we show that the entanglement of the state obtained by beam splitting of one occupied mode is fully inherited from sub-Poissonian statistics of the input state.

2. Mesoscopic description of bosonic modes

One of the crucial quantum phenomena is entanglement, which is one of the core resources in many quantum information tasks. This is even more so since in the quantum field theory the entanglement of pure states is fundamentally associated with Bell non-classicality [25], which is necessary for device-independent quantum key distribution. For such tasks, particularly compelling is the encoding of information in light modes, as light can be quickly distributed over long distances [16]. What is more, fully photonic quantum devices are one of the promising avenues also in different subfields of quantum information, e.g. quantum computing [26]. However, as all quantum systems, light modes are also affected by the environment and undergo non-unitary open evolution. This results in decoherence of the system and thus decay of quantum phenomena such as superposition (including entanglement).

In general, the full description of a non-unitary evolution of the state in terms of infinite-dimensional Fock space can be cumbersome or even infeasible. This is especially true for complicated mesoscopic systems that involve multiple bosonic modes occupied by an undefined number of particles. A custom in the treatment of mesoscopic systems is to consider only some degrees of freedom instead of the full quantum state of the field $\hat{\rho}_F$. This allows for reducing the complexity of the problem. One of such methods for bosonic systems is to track the evolution of the covariance matrix of position and momenta [19]:

$$V_{i,j} = \frac{1}{2}\langle\left\{\hat{\Xi}_i, \hat{\Xi}_j\right\}\rangle - \langle\hat{\Xi}_i\rangle\langle\hat{\Xi}_j\rangle, \tag{1}$$

where $\vec{\Xi} = (\hat{x}_1, \hat{p}_1, \ldots, \hat{x}_N, \hat{p}_N)$, and operators $\hat{x}_j, \hat{p}_j$ are dimensionless position and momentum operators in jth mode, respectively. This method is particularly important, as it allows tracking of the full Gaussian evolution of Gaussian states. The reason for this is that one can reconstruct the full Gaussian state $\hat{\rho}_F$ from the covariance matrix. Therefore, the covariance matrix also contains full information about the entanglement of Gaussian states, which in the case of distillable bipartite entanglement can be accessed simply by using the PPT criterion [3, 27, 28]. However, this is not always the case for non-Gaussian states, e.g. cat-like states. For such states, one has to employ different methods of entanglement detection for which information contained in the covariance matrix is not sufficient [20]. Furthermore, the covariance matrix approach, while well suited for continuous variable analysis, can be non-intuitive with its symplectic structures. This may particularly concern researchers for researchers working solely with discrete variables, for whom finite-dimensional Hilbert spaces of the first quantization equipped with the Dirac notation can be more familiar. Additionally, regaining information from the covariance matrix about discrete variables also requires extra effort, and it is not always possible for non-Gaussian states.

In fact, multiple fundamental experiments and protocols, e.g. teleportation [29], entanglement swapping [30], and quantum cryptography [31] are based on entanglement of qubits realized using light modes restricted to a single photon per party. Emblematic examples of the states used in such protocols are polarization and path-entangled singlet states. Denoting by $\hat{a}_j^\dagger$ the creation operator in $j$the mode and vacuum state by $|\Omega\rangle$, such states can be written as:

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(\hat{a}_1^\dagger\hat{a}_4^\dagger - \hat{a}_2^\dagger\hat{a}_3^\dagger\right)|\Omega\rangle = \frac{1}{\sqrt{2}}\left(|1,0;0,1\rangle - |0,1;1,0\rangle\right). \tag{2}$$

Here, one chooses partition into two parties (subsystems), such that polarization or path modes a_1, a_2 are associated with one party and modes a_3, a_4 with the second one. Here we have also used the following notation for Fock states:

$$|n_1, n_2; n_3, n_4\rangle = \frac{\left(\hat{a}_1^\dagger\right)^{n_1}\left(\hat{a}_2^\dagger\right)^{n_2}\left(\hat{a}_3^\dagger\right)^{n_3}\left(\hat{a}_4^\dagger\right)^{n_4}}{\sqrt{n_1!n_2!n_3!n_4!}}|\Omega\rangle, \tag{3}$$

with semicolon marking the bipartition. Then, the measurements that correspond to Pauli matrices typically considered for qubits are realized as Stokes operators $\hat{\Theta}_i$ [32] restricted to the single-photon subspace:

$$\sigma_i \to \hat{\Pi}_1\hat{\Theta}_i\hat{\Pi}_1 = \hat{\Pi}_1\left(\hat{a}_i^\dagger\hat{a}_i - \hat{a}_{i_\perp}^\dagger\hat{a}_{i_\perp}\right)\hat{\Pi}_1, \tag{4}$$

where $i = 1,2,3$ denotes one of the three mutually unbiased basis described by two orthogonal modes $a_i, a_{i\perp}$, and $\hat{\Pi}_1$ stands for the projector into the subspace of single photon across these modes. Additionally, after projecting with $\hat{\Pi}_1$, the total photon number operator $\Theta_0 = \hat{a}_i^\dagger\hat{a}_i + \hat{a}_{i_\perp}^\dagger\hat{a}_{i_\perp}$ corresponds to the identity on the qubit space denoted by σ_0. Note that any local operation on the two-qubit system can be described as a combination of tensor products of Pauli matrices (including σ_0) acting on subsystems A and B. In the Fock space, this translates to $\sigma_i^A \otimes \sigma_j^B \to \hat{\Pi}_1^A\hat{\Pi}_1^B\hat{\Theta}_i^A\hat{\Theta}_j^B\hat{\Pi}_1^B\hat{\Pi}_1^A$, where upper indices denote the party on which the given operators act. Therefore, as Stokes operators are, in fact, differences of number operators in two orthogonal modes, all non-classical correlations in such systems are described as photon number correlations $\langle(\hat{a}_{i(\perp)}^A)^\dagger\hat{a}_{i(\perp)}^A(\hat{a}_{j(\perp)}^B)^\dagger\hat{a}_{j(\perp)}^B\rangle$. This suggests that boson number entanglement is at the core of the discrete variable bipartite entanglement of bosonic systems. What is more, such correlations also become experimentally accessible in regimes with higher photon numbers due to developments in the field of photon number resolving detectors [33, 34]. Let us note that the considered photonic implementation of qubits is, in fact, approximate. This is because nothing prevents the given modes from being occupied by a higher or lower number of photons. It is an issue even with event-ready preparation of the system in which a photon is confirmed to enter the input of the apparatus, as the environment can add multi-photon noise (with an undefined number of photons) or cause loss of the photon which encodes the information. Such a problem arises especially during propagation through long transmission lines. Thus, even in these highly simplified scenarios, in principle, one should consider the full Fock space, or at least consider some mesoscopic description of the system. All of this motivates us to build a mesoscopic scale description of bosonic systems with the following matrix as the main structure that contains relevant degrees of freedom of the state $\hat{\rho}_F$ for considerations of bipartite entanglement:

$$\hat{\rho}_4 := \sum_{i,j,n,m}^{N} \mathrm{tr}\,\hat{\rho}_F\hat{a}_n^\dagger\hat{a}_i\hat{a}_m^\dagger\hat{a}_j|i,j\rangle\langle n,m|. \tag{5}$$

In the following, we show that $\hat{\rho}_4$, which we call *extended reduced state*, contains information about entanglement of both Gaussian states with high average numbers of particles, and more importantly, non-Gaussian states (for which the PPT criterion cannot reveal entanglement based on the covariance matrix). At the same time, we equip the proposed mesoscopic description with multiple intuitive and familiar tools from finite-dimensional Hilbert spaces.

Furthermore, in many circumstances, the open evolution imposed on the system is approximately Markovian. Thus, further on we show the set of evolution equations for the matrix $\hat{\rho}_4$ for such scenarios. This type of evolution of the full state of the bosonic modes $\hat{\rho}_F$ is described by the GKLS equation [35, 36]. In particular, this equation can be written for N orthogonal bosonic modes a_j using the independent particles approximation in such a way that it includes relevant processes of particle decay and production, random elastic scattering, and classical coherent pumping [21, 24]. We base our considerations upon this equation, which reads:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_F = & -\frac{i}{\hbar}\left[\hat{H},\rho_F\right] + \sum_k^N \left[\left(\xi_k \hat{a}_k^\dagger - \xi_k^* \hat{a}_k\right),\hat{\rho}_F\right] + \sum_j \kappa_j \left(\hat{U}_j \hat{\rho}_F \hat{U}_j^\dagger - \hat{\rho}_F\right) \\ & + \sum_{k,k'=1}^N \Gamma_\downarrow^{k',k}\left(\hat{a}_k \hat{\rho}_F \hat{a}_{k'}^\dagger - \frac{1}{2}\left\{\hat{a}_{k'}^\dagger \hat{a}_k, \hat{\rho}_F\right\}\right) + \sum_{k,k'=1}^N \Gamma_\uparrow^{k',k}\left(\hat{a}_{k'}^\dagger \hat{\rho}_F \hat{a}_k - \frac{1}{2}\left\{\hat{a}_k \hat{a}_{k'}^\dagger, \hat{\rho}_F\right\}\right),\end{aligned} \tag{6}$$

with Hamiltonian $\hat{H} = \sum_{k,k'} \omega_{k,k'} \hat{a}_k^\dagger \hat{a}_{k'}$, where $\hat{a}_k^\dagger (\hat{a}_k)$ are creation (annihilation) operators associated with corresponding modes, complex parameters ξ_k describe classical pumping field, $\hat{U}_j$ are unitary transformations of annihilation operators ($\hat{U}_j^\dagger \hat{a}_k \hat{U}_j = \sum_{k'} u_{k',k}^j \hat{a}_{k'}$ with u^j being unitary matrix) corresponding to scattering processes with their probability distribution κ_j, and $\Gamma_\uparrow^{k',k}$ ($\Gamma_\downarrow^{k',k}$) describe creation (annihilation) rate.

3. Separability in terms of extended reduced state

The key question for entanglement considerations in our mesoscopic description is how separability in the Fock space translates into the extended reduced state. The following considerations are inspired by the mappings of the entanglement indicators for Stokes-like operators [37, 38]. Let us choose two sets of indices $\mathcal{I}_A, \mathcal{I}_B \in \{1, N\}$ in such a way that $\mathcal{I}_A \cap \mathcal{I}_B = \varnothing$, which determines our bipartition of the system. We assume that the modes with indices from $\mathcal{I}_A$ constitute one subsystem and the modes with indices from $\mathcal{I}_B$ the second one. In addition, each set contains at least two elements, and we denote the number of these elements by $d_X = \overline{\mathcal{I}_X}$. Based on this choice, we project the operator $\hat{\rho}_4$ in the following way:

$$\hat{\rho}_4 \to \hat{\rho}^\Pi = \hat{\Pi}_{\mathcal{I}_A,\mathcal{I}_B} \hat{\rho}_4 \hat{\Pi}_{\mathcal{I}_A,\mathcal{I}_B} = \sum_{i,n\in\mathcal{I}_A} \sum_{j,m\in\mathcal{I}_B} \rho_{ijnm} |i,j\rangle\langle n,m|, \tag{7}$$

where:

$$\Pi_{\mathcal{I}_A,\mathcal{I}_B} = \sum_{i\in\mathcal{I}_A} \sum_{j\in\mathcal{I}_B} |i,j\rangle\langle i,j|, \tag{8}$$

and $\rho_{ijnm} = \langle \hat{a}_n^\dagger \hat{a}_i \hat{a}_m^\dagger \hat{a}_j \rangle$ are corresponding matrix elements of $\hat{\rho}_4$. Let us here for clarity rename the operators corresponding to modes $\mathcal{I}_B$ as $\hat{b}_m^\dagger$ and $\hat{b}_j$, i.e. $\langle \hat{a}_n^\dagger \hat{a}_i \hat{a}_m^\dagger \hat{a}_j \rangle \to \langle \hat{a}_n^\dagger \hat{a}_i \hat{b}_m^\dagger \hat{b}_j \rangle$. Note that the modes that are not used are effectively traced out and modes from $\mathcal{I}_A$ ($\mathcal{I}_B$) are associated only with the first (second) index of the kets and bras.

Let us assume that the state of the system $\hat{\rho}_F$ after tracing out modes not contained in $\mathcal{I}_A, \mathcal{I}_B$ is some pure state $\hat{\rho}_F = |\psi\rangle\langle\psi|$. In such a case, we can see that ρ_{ijnm} has the form:

$$\rho_{ijnm} = \langle \psi_{nm} | \psi_{ij} \rangle, \tag{9}$$

where $|\psi_{ij}\rangle = \hat{a}_i \hat{a}_j |\psi\rangle$. From this it follows that ρ_{ijnm} forms a Gramian matrix and thus is positive definite. Thus $\hat{\rho}_\psi^\Pi$ (where the subscript denotes the original state on the Fock space) is also positive definite, and after normalization it is a well-defined density matrix $\hat{\rho}_\psi^\mathcal{N}$ for the system of two qudits with respective dimensions d_X. However, there are exceptions for which the matrix cannot be normalized, as it is traceless. The trace of this matrix is equal to $\langle \hat{N}_{\mathcal{I}_A} \hat{N}_{\mathcal{I}_B} \rangle$ where $\hat{N}_{\mathcal{I}_X}$ is the total boson number operator in modes corresponding to $\mathcal{I}_X$. This can be zero only when the state is the vacuum $\hat{\rho}_F = |\Omega\rangle\langle\Omega|$ or when in the superposition it consists only of states with bosons only in one subsystem. We address this problem later on. For now, assume that the matrix can be normalized. Because any mixed state can be written as a convex combination of pure states $\hat{\rho}_F = \sum_i p_i |\phi_i\rangle\langle\phi_i|$, it maps to a convex combination of $\hat{\rho}_{\phi_i}^\Pi$:

$$\hat{\rho}_{\rho_F}^\Pi = \sum_i p_i \hat{\rho}_{\phi_i}^\Pi. \tag{10}$$

After normalization, we get:

$$\hat{\rho}^{\mathcal{N}}_{\rho_F} = \sum_i p_i \hat{\rho}^{\Pi}_{\phi_i} / \sum_i p_i \operatorname{tr} \hat{\rho}^{\Pi}_{\phi_i} = \sum_i p_i \operatorname{tr} \hat{\rho}^{\Pi}_{\phi_i} \hat{\rho}^{\mathcal{N}}_{\phi_i} / \sum_i p_i \operatorname{tr} \hat{\rho}^{\Pi}_{\phi_i} = \sum_i p'_i \hat{\rho}^{\mathcal{N}}_{\phi_i}. \tag{11}$$

Note that $1 \leqslant p'_i \leqslant 0$ and $\sum_i p'_i = 1$. Thus, this again forms a proper density matrix on the two-qudit space.

In the next step, we assume that $\hat{\rho}_F$ is separable in the partition into modes $\mathcal{I}_A$ and $\mathcal{I}_B$. We start with the case where $\hat{\rho}_F$ is in some pure state $|\psi\rangle\langle\psi|$. Due to separability, the state can be written as $|\psi\rangle = F^{\dagger}_{\mathcal{I}_A} F^{\dagger}_{\mathcal{I}_B}|\Omega\rangle$, where $|\Omega\rangle$ stands for vacuum state, and $F^{\dagger}_{\mathcal{I}_i}$ is a polynomial of creation operators of modes corresponding to $\mathcal{I}_X$. From this follows that each ρ_{ijnm} from $\hat{\rho}^{\Pi}$ factorizes as follows:

$$\begin{aligned}\rho_{ijnm} &= \langle\Omega|F_{\mathcal{I}_A} F_{\mathcal{I}_B} \hat{a}^{\dagger}_n \hat{a}_i \hat{b}^{\dagger}_m \hat{b}_j F^{\dagger}_{\mathcal{I}_A} F^{\dagger}_{\mathcal{I}_B}|\Omega\rangle \\ &= \langle\Omega|F_{\mathcal{I}_A} \hat{a}^{\dagger}_n \hat{a}_i F^{\dagger}_{\mathcal{I}_A}|\Omega\rangle\langle\Omega|F_{\mathcal{I}_B} \hat{b}^{\dagger}_m \hat{b}_j F^{\dagger}_{\mathcal{I}_B}|\Omega\rangle = \langle\psi^A_n|\psi^A_i\rangle\langle\psi^B_m|\psi^B_j\rangle,\end{aligned} \tag{12}$$

where $|\psi^A_i\rangle = \hat{a}_i F^{\dagger}_{\mathcal{I}_A}|\Omega\rangle$ and $|\psi^B_j\rangle = \hat{b}_j F^{\dagger}_{\mathcal{I}_B}|\Omega\rangle$. To see this, consider a rearrangement of the creation and annihilation operators in ρ_{ijnm} such that the operators corresponding to $\mathcal{I}_B$ are shifted to the right. Let us then put the resolution of identity $\mathbb{1} = \sum_{\vec{n}_1,\vec{n}_2} |\vec{n}_1;\vec{n}_2\rangle\langle\vec{n}_1;\vec{n}_2|$ between the operators acting on the modes $\mathcal{I}_A$ and $\mathcal{I}_B$. This results in:

$$\begin{aligned}\rho_{ijnm} &= \langle\Omega|F_{\mathcal{I}_A} \hat{a}^{\dagger}_n \hat{a}_i F^{\dagger}_{\mathcal{I}_A} \mathbb{1} F_{\mathcal{I}_B} \hat{b}^{\dagger}_m \hat{b}_j F^{\dagger}_{\mathcal{I}_B}|\Omega\rangle = \langle\Omega|F_{\mathcal{I}_A} \hat{a}^{\dagger}_n \hat{a}_i F^{\dagger}_{\mathcal{I}_A}|\Omega\rangle\langle\Omega|F_{\mathcal{I}_B} \hat{b}^{\dagger}_m \hat{b}_j F^{\dagger}_{\mathcal{I}_B}|\Omega\rangle \\ &+ \sum_{\vec{n}_1 \neq \vec{0}} \langle\Omega|F_{\mathcal{I}_A} \hat{a}^{\dagger}_n \hat{a}_i F^{\dagger}_{\mathcal{I}_A}|\vec{n}_1;\vec{0}\rangle\langle\vec{n}_1;\vec{0}|F_{\mathcal{I}_B} \hat{b}^{\dagger}_m \hat{b}_j F^{\dagger}_{\mathcal{I}_B}|\Omega\rangle \\ &+ \sum_{\vec{n}_2 \neq \vec{0}} \langle\Omega|F_{\mathcal{I}_A} \hat{a}^{\dagger}_n \hat{a}_i F^{\dagger}_{\mathcal{I}_A}|\vec{0};\vec{n}_2\rangle\langle\vec{0};\vec{n}_2|F_{\mathcal{I}_B} \hat{b}^{\dagger}_m \hat{b}_j F^{\dagger}_{\mathcal{I}_B}|\Omega\rangle \\ &+ \sum_{\vec{n}_1,\vec{n}_2 \neq \vec{0}} \langle\Omega|F_{\mathcal{I}_A} \hat{a}^{\dagger}_n \hat{a}_i F^{\dagger}_{\mathcal{I}_A}|\vec{n}_1;\vec{n}_2\rangle\langle\vec{n}_1;\vec{n}_2|F_{\mathcal{I}_B} \hat{b}^{\dagger}_m \hat{b}_j F^{\dagger}_{\mathcal{I}_B}|\Omega\rangle,\end{aligned} \tag{13}$$

where $|\vec{n}_1;\vec{n}_2\rangle$ stands for the Fock basis state with occupancy of the modes $\mathcal{I}_A$ and $\mathcal{I}_B$ described by vectors $\vec{n}_1, \vec{n}_2$, and $\vec{0}$ stands for 0 photons in given modes. This rearrangement is possible as operators acting on orthogonal modes $\mathcal{I}_A$ and $\mathcal{I}_B$ commute. One can notice that terms of the first sum appearing in (13) contain factor $\langle\vec{n}_1;\vec{0}|F_{\mathcal{I}_B} \hat{a}^{\dagger}_m \hat{a}_j F^{\dagger}_{\mathcal{I}_B}|\Omega\rangle$ which is equal to 0. This is because all operators inside the expectation value act only on modes $\mathcal{I}_B$ leaving part of the bra and ket corresponding to modes $\mathcal{I}_A$ orthogonal. Analogously, all other sums that appear in (13) are equal to 0, and the relation is proven. Now, based on the same arguments as above, $\rho^X_{\psi,l,k} := \langle\psi^X_k|\psi^X_l\rangle$ forms a proper density matrix after normalization on the one-qudit space. Thus, $\hat{\rho}^{\mathcal{N}}_{\psi} = \hat{\rho}^1_{\psi} \otimes \hat{\rho}^2_{\psi}/\mathcal{N}$ is a separable state on the two-qudit space. For the mixed separable state, we see from (11) that $\hat{\rho}^{\mathcal{N}}_{\rho_F}$ is a convex combination of pure separable states and therefore a proper separable mixed state on the two-qudit space. Therefore, if $\hat{\rho}^{\mathcal{N}}_{\rho_F}$ is entangled, then $\hat{\rho}_F$ is entangled.

Let us now address the scenario in which the matrix for the pure state is not normalizable. This was not important for mapping of entanglement indicators [37, 38]. However, it is important if one wants to use $\hat{\rho}^{\mathcal{N}}_{\rho_F}$ in a more general context as a density operator. All pure states that result in the not normalizable $\hat{\rho}^{\Pi}_{\psi}$ have the following form:

$$|\psi\rangle = \zeta_0|\Omega\rangle + F^{\dagger}_{\mathcal{I}_A}|\Omega\rangle + F^{\dagger}_{\mathcal{I}_B}|\Omega\rangle, \tag{14}$$

where ζ_0 stands for amplitude of vacuum state. These states can be either separable or entangled. One can easily find that for all such states $\hat{\rho}^{\Pi}_{\psi} = 0$. This tells us that for states of the form (14) this state reduction does not allow one to access the information about their entanglement without some additional considerations. What is more, all of them are equivalent to vacuum (which is separable) at the level of reduction to $\hat{\rho}^{\Pi}_{\psi}$. Despite that, there is a way to gain access to the entanglement of such states in our description. We discuss this further in examples. Note that such states are effectively highly unlikely to be present in experiments due to the presence of noise, for example, thermal noise. Therefore, the important question is the impact of such states if they are part of the mixed state $\hat{\rho}_F$. Without loss of generality, assume that only $|\phi_0\rangle$ is of the form (14):

$$\hat{\rho}^{\Pi}_{\rho_F} = p_0 \hat{0} + \sum_{i \geqslant 1} p_i \hat{\rho}^{\Pi}_{\phi_i} \rightarrow \hat{\rho}^{\mathcal{N}}_{\rho_F} = \sum_{i \geqslant 1} p_i \operatorname{tr} \hat{\rho}^{\Pi}_{\phi_i} \hat{\rho}^{\mathcal{N}}_{\phi_i} / \sum_{i \geqslant 1} p_i \operatorname{tr} \hat{\rho}^{\Pi}_{\phi_i} = \sum_{i \geqslant 1} p''_i \hat{\rho}^{\mathcal{N}}_{\phi_i}, \tag{15}$$

where p''_i fulfill relations for probability. Therefore, even in this case $\hat{\rho}^{\mathcal{N}}_{\rho_F}$ is a well-defined density matrix, and clearly the previous discussion on separability holds. In fact, the presence of the states (14) in the density matrix results only in renormalization of probabilities and thus neither helps to detect entanglement nor prevents it. One can observe that all states of the form:

$$\hat{\rho}_F = p_1 \sum_j q_j |\psi_j\rangle\langle\psi_j| + p_2 \hat{\rho}', \tag{16}$$

with $|\psi_j\rangle$ having the form (14) and q_j, p_i being independent probability distributions, are equivalent to the state $\hat{\rho}'$ in terms of $\hat{\rho}^{\mathcal{N}}_{\rho_F}$.

Note that separability of $\hat{\rho}^{\Pi}_{\psi}$ does not imply that $\hat{\rho}_F$ is separable, since we use only part of the correlations. In other words, the entanglement of the state $\hat{\rho}^{\Pi}_{\psi}$ on the reduced two-qudit Hilbert space is a sufficient condition for the entanglement of $\hat{\rho}_F$. Importantly, one has to consider at least 4 modes to reveal such a kind of entanglement, as one has to have both reduced subsystems at least two-dimensional.

3.1. Impact of mode transformations

Note that the choice of the basis in the subsystem defined by $\mathcal{I}_i$ has no impact on the detection of entanglement. This is because the local unitary transformation of the annihilation operators that constitutes a basis transformation translates into the local change of basis in the reduced matrix ρ^{Π}. Let us consider a general form of such a transformation $\hat{a}_i = \sum_k U_{ik}\hat{c}_k$, where $\hat{c}_k$ are annihilation operators in some new basis, and U_{ik} determines the transformation between bases. Let us consider a transformation in the first subsystem:

$$\rho^{(a)}_{ijnm} = \langle\psi|\hat{a}^\dagger_n \hat{b}^\dagger_m \hat{a}_i \hat{b}_j|\psi\rangle = \sum_{k,l} U_{i,k}\langle\psi|\hat{c}^\dagger_l \hat{b}^\dagger_m \hat{c}_k \hat{b}_j|\psi\rangle U^*_{l,n} = \sum_{k,l} U_{i,k}\rho^{(c)}_{kjlm} U^*_{l,n}, \tag{17}$$

where the superscript in $\rho^{(a)}_{ijnm}$ denotes the basis used. This transformation is simply a basis transformation on the subsystem. Such transformations do not affect the separability of the state.

From this we see that by choice of partition of modes our reduction procedure maps boson number entanglement into the entanglement of two distinguishable particles with finite number of levels. The extended reduced state $\hat{\rho}_4$ contains information about all partitions $\mathcal{I}_A, \mathcal{I}_B$. Thus, the separability of $\hat{\rho}^{\mathcal{N}}_{\rho_F}$ for one partition does not necessarily mean that $\hat{\rho}_4$ does not contain any information on the entanglement. In fact, $\hat{\rho}_4$ contains information about the boson number entanglement in any partition $\mathcal{I}_A, \mathcal{I}_B$ after an arbitrary unitary basis transformation of all modes, which can be seen analogously to (17). Still, sensible partitions easily emerge in the experimental setups, where specific modes correspond to different beams clearly determining local operations.

4. Open evolution and reduced state of the field approach

In the previous section, we effectively mapped the relevant in the context of entanglement degrees of freedom of a state $\hat{\rho}_F$ from the infinite-dimensional Fock space into the mixed state $\hat{\rho}^{\mathcal{N}}_{\rho_F}$ on two-particle-like finite-dimensional Hilbert space. It is important to note that while $\hat{\rho}^{\mathcal{N}}_{\rho_F}$ possesses all mathematical features of the density matrix, it does not inherit a probabilistic interpretation of the entries on the diagonal of the matrix. Here, they describe the strength of linear correlations of boson numbers between given modes. This situation is similar to the case of the RSF approach to the mesoscopic description of bosonic modes [21]. In fact, our reduction can be seen as a higher-order extension of the RSF.

Let us briefly recall the RSF approach. The RSF formalism attempts to reduce the infinite-dimensional description of the second quantization into a single-particle-like finite-dimensional Hilbert space of the first quantization. This reduction is carried out as follows. Consider a density operator $\hat{\rho}_F$ on the Fock space that describes the state of N orthogonal modes $\{a_k\}_{k=1}^N$. This operator is reduced to two structures on the N-dimensional Hilbert space equipped with orthonormal basis $\{|k\rangle\}_{k=1}^N$, single-particle density matrix and averaged field:

$$\hat{\rho} = \sum_{k,k'=1}^{N} \mathrm{tr}\,\hat{\rho}_F \hat{a}^\dagger_{k'}\hat{a}_k |k\rangle\langle k'|, \quad |\alpha\rangle = \sum_{k=1}^{N} \mathrm{tr}\,\hat{\rho}_F \hat{a}_k |k\rangle. \tag{18}$$

The operator $\hat{\rho}$ contains information on the occupation of modes and coherences, while $|\alpha\rangle$ about the local phases of the field. Note that $\hat{\rho}$ and $|\alpha\rangle$ after normalization have the properties of a density matrix and a pure state, respectively; however, they do not inherit the probabilistic interpretation normally associated with quantum states. One can see that the diagonal elements of $\hat{\rho}$ represent the average occupation of modes instead of probabilities. The reduction of the state is also accompanied by a reduction of observables. One can reduce a class of additive observables on the Fock space in the following way:

$$\hat{O} = \sum_{k,k'=1}^{N} o_{k,k'} a_k^\dagger \hat{a}_{k'} \to \hat{o} = \sum_{k,k'=1}^{N} o_{k,k'} |k\rangle\langle k'|. \tag{19}$$

This construction preserves the expectation values:

$$\mathrm{tr}\,\hat{\rho}_F \hat{O} = \mathrm{tr}\,\hat{\rho}\hat{o}. \tag{20}$$

What is important, one can find the time evolution equations for $\hat{\rho}$, $|\alpha\rangle$ corresponding to the evolution equation (6):

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho} = -\frac{i}{\hbar}\left[\hat{h},\hat{\rho}\right] + (|\xi\rangle\langle\alpha| + |\alpha\rangle\langle\xi|) + \sum_j \kappa_j \left(\hat{u}_j \hat{\rho}\hat{u}_j^\dagger - \hat{\rho}\right) + \frac{1}{2}\{\hat{\gamma}_\uparrow - \hat{\gamma}_\downarrow^T, \hat{\rho}\} + \hat{\gamma}_\uparrow, \tag{21}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}|\alpha\rangle = -\frac{i}{\hbar}\hat{h}|\alpha\rangle + |\xi\rangle + \sum_j \kappa_j \left(\hat{u}_j - 1\right)|\alpha\rangle + \frac{1}{2}\left(\hat{\gamma}_\uparrow - \hat{\gamma}_\downarrow^T\right)|\alpha\rangle, \tag{22}$$

where $\hat{h}$ stands for reduced Hamiltonian (using (19)), and:

$$\hat{\gamma}_\updownarrow = \sum_{k,k'} \Gamma_\updownarrow^{kk'} |k\rangle\langle k'|, \quad |\xi\rangle = \sum_k \xi_k |k\rangle, \quad \hat{u}_j = \sum_{k,k'} u_{k,k'}^j |k\rangle\langle k'|. \tag{23}$$

This formalism is also equipped with notion of entropy:

$$S[\hat{\rho};|\alpha\rangle] = k_\mathrm{B}\,\mathrm{tr}\,(\hat{\rho}^\alpha + 1)\log(\hat{\rho}^\alpha + 1) - \hat{\rho}^\alpha \log(\hat{\rho}^\alpha), \tag{24}$$

where k_B stands for Boltzmann constant, and $\hat{\rho}^\alpha = \hat{\rho} - |\alpha\rangle\langle\alpha|$.

4.1. Extended reduced state of the field description

The RSF formalism, while simple, has drawbacks limiting its applications. Although it is fully based on quantum considerations, it is a highly classical description [24]. This is in the sense that RSF does not contain information about non-classical phenomena like distillable entanglement. Therefore, it was conjectured that RSF does not contain any information on entanglement, which was strictly shown for two-mode Gaussian states. What is more, the entropy of this formalism has properties similar to the semi-classical Wehrl entropy rather than the quantum von Neumann entropy. However, it turns out that the information contained in RSF is needed to track the evolution of our *reduced two-particle-like state* $\hat{\rho}_{\rho_F}^{\mathcal{N}}$. Moreover, this evolution can be put into a framework that extends RSF in a natural way. This extension can be seen as the simplest extension of RSF that adds quantum features to the formalism and is not equivalent to the covariance matrix formalism.

Let us show how our extended reduced state $\hat{\rho}_4$ can be incorporated into an RSF-like formalism. States from the single-particle space of RSF contain information about particle numbers in modes. Thus, a natural concept is to introduce a tensor product of two single-particle spaces to track correlations of particle numbers. The extended reduced state $\hat{\rho}_4$ is then an operator on the two-particle Hilbert space constructed based on two copies of the single-particle space. Note that reduction of state $\hat{\rho}_F$ does not always have to result in the operator $\hat{\rho}_4$ being Hermitian. Thus, it does not have to constitute a proper state on this Hilbert space, but still $\hat{\rho}_{\rho_F}^{\mathcal{N}}$ does. We keep the whole structure $\hat{\rho}_4$ as it provides additional useful information on quantum features of the state. We will exploit this information later. Moreover, $\hat{\rho}_4$ is necessary for deriving a closed set of evolution equations that corresponds to (6). We build an extended reduced state $\hat{\rho}_4$ (5) to resemble a single-particle density matrix $\hat{\rho}$ (18), i.e. with indices of annihilation operators responsible for labeling rows and indices of creation operators labeling columns. Analogously to (19), one can reduce the observables:

$$\hat{O}_4 = \sum_{k_1,k_2,k_3,k_4} o_{k_1,k_2,k_3,k_4} \hat{a}_{k_1}^\dagger \hat{a}_{k_2} \hat{a}_{k_3}^\dagger \hat{a}_{k_4} \to \hat{o}_4 = \sum_{k_1,k_2,k_3,k_4} o_{k_1,k_2,k_3,k_4} |k_1,k_3\rangle\langle k_2,k_4|, \tag{25}$$

with $\mathrm{tr}\,\hat{\rho}_F\hat{O}_4 = \mathrm{tr}\,\hat{\rho}_4\hat{o}_4$. We also complement the reduction of the state with two additional structures, a rank 3 tensor:

$$\hat{\beta} := \sum_{k_1,k_2,k_3,k_4} \mathrm{tr}\,\hat{\rho}_F \hat{a}_{k_1}^\dagger \hat{a}_{k_2} \hat{a}_{k_3} |k_2,k_3\rangle\langle k_1|, \tag{26}$$

and an additional operator on single-particle space:

$$\hat{r} = \sum_{k,k'} \mathrm{Tr}\, \hat{\rho}_F \hat{a}_{k'} \hat{a}_k |k\rangle\langle k'|. \tag{27}$$

These two structures are introduced solely in order to include coherent pumping in the evolution, which will become apparent from the evolution equations. The evolution of operators on two-particle space also requires tracking the evolution in a single-particle space. Thus, this two-particle reduction has to be used together with the single-particle reduction, and the *total reduced state* consists of $\hat{\rho}_4, \hat{\beta}, \hat{r}, \hat{\rho}, |\alpha\rangle$. The Markovian evolution equations for operators $\hat{\rho}_4$, $\hat{\beta}$, $\hat{r}$ can be obtained analogously to equations (21) and (22). This is achieved by multiplying both sides of (6) with a suitable combination of creation and annihilation operators for a given matrix element and then tracing the resulting expressions. Then, after some simplifications done with the commutation relation $[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}$, the set of evolution equations can be put in the following form:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_4 = & -\frac{i}{\hbar}\left[\hat{h}\otimes\mathbf{1}+\mathbf{1}\otimes\hat{h}, \hat{\rho}_4\right] + \left(|\xi\rangle\hat{\beta}^\dagger + \left(|\xi\rangle\hat{\beta}^\dagger\right)^{\tau_L} + \left(|\xi\rangle\langle\alpha|\otimes\mathbf{1}\right)^{\tau_L} + \hat{\beta}\langle\xi| + \left(\hat{\beta}\langle\xi|\right)^{\tau_R} + \left(\mathbf{1}\otimes|\alpha\rangle\langle\xi|\right)^{\tau_R}\right) \\ & + \sum_j \kappa_j\left(\hat{u}_j\otimes\hat{u}_j\hat{\rho}_4\hat{u}_j^\dagger\otimes u_j^\dagger - \hat{\rho}_4\right) + \frac{1}{2}\{(\mathbf{1}\otimes\hat{\gamma}_\uparrow + \hat{\gamma}_\uparrow\otimes\mathbf{1}) - \left(\mathbf{1}\otimes\hat{\gamma}_\downarrow^T + \hat{\gamma}_\downarrow^T\otimes\mathbf{1}\right), \hat{\rho}_4\} \\ & + \left(\hat{\rho}\otimes\gamma_\downarrow^T\right)^{\tau_L} + \left(\gamma_\uparrow\otimes\hat{\rho}\right)^{\tau_L} + \gamma_\uparrow\otimes\hat{\rho} + \hat{\rho}\otimes\gamma_\uparrow + \left(\gamma_\uparrow\otimes\mathbf{1}\right)^{\tau_L},\end{aligned} \tag{28}$$

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\hat{\beta} = & -\frac{i}{\hbar}\left[\hat{h}\otimes\mathbf{1}, \hat{\beta}\right] - \frac{i}{\hbar}\mathbf{1}\otimes\hat{h}\hat{\beta} + \left(\hat{\rho}\otimes|\xi\rangle + \left(\hat{\rho}\otimes|\xi\rangle\right)^{\tau_L} + \left[\left(\hat{r}\otimes\langle\xi|\right)^{\tau_R}\right]^{T_2}\right) + \sum_j \kappa_j\left(\hat{u}_j\otimes\hat{u}_j\hat{\beta}\hat{u}_j^\dagger - \hat{\beta}\right) \\ & + \frac{1}{2}\left(\{\hat{\gamma}_\uparrow\otimes\mathbf{1} - \hat{\gamma}_\downarrow^T\otimes\mathbf{1}, \hat{\beta}\} + \left(\mathbf{1}\otimes\hat{\gamma}_\uparrow - \mathbf{1}\otimes\hat{\gamma}_\downarrow^T\right)\hat{\beta}\right) + \hat{\gamma}_\uparrow\otimes|\alpha\rangle + \left(\hat{\gamma}_\uparrow\otimes|\alpha\rangle\right)^{\tau_L}\end{aligned} \tag{29}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{r} = -\frac{i}{\hbar}\hat{h}\hat{r} + |\xi\rangle\langle\alpha^*| + \frac{1}{2}\left(\hat{\gamma}_\uparrow - \hat{\gamma}_\downarrow^T\right)\hat{r} + T. + \sum_j \kappa_j\left(\hat{u}_j\hat{r}\hat{u}_j^T - \hat{r}\right). \tag{30}$$

Here, we introduced the following notation: T_i stands for transposition on ith space, τ_L acts on kets as follows $|n,m\rangle \to |m,n\rangle$ and τ_R acts analogously on bras, and '$T.$' stands for the transposed expression. Also, for some operator on single-particle space $\hat{o}$, we denote $|k_2,k_3\rangle\langle k_1|\hat{o}\otimes\mathbf{1} := |k_2,k_3\rangle\langle k_1|\hat{o}$, and $|k_2\rangle\langle k_3|\otimes|k_1\rangle := |k_2,k_1\rangle\langle k_3|$, and $|k_2,k_3\rangle\langle k_1|\langle k_4| := |k_2,k_3\rangle\langle k_1,k_4|$. One can observe that if there is no coherent pumping (i.e. $\forall_i \xi_i = 0$), evolution of the operators $\hat{\rho}_4$ and $\hat{\rho}$ decouples from evolution of the rest of the operators. Therefore, in such circumstances, $\hat{\rho}_4$ and $\hat{\rho}$ can be considered by themselves without considering $\hat{\beta}$ and $\hat{r}$, for which there is a lack of a quantum state-like interpretation. Note that the first term of the evolution equation (28) for $\hat{\rho}_4$ resembles the Heisenberg equation, and it is responsible for the unitary evolution generated by the Hamiltonian. The remaining terms come from decoherence and pumping terms, as in the case of $\hat{\rho}$. Let us also comment that $\hat{r}$ together with $\hat{\rho}$ and $|\alpha\rangle$ allow for reconstruction of the covariance matrix. Therefore, the extension of RSF by $\hat{r}$ is the simplest extension of RSF that gives quantum features to this formalism. However, it is trivial in the sense that it reproduces the covariance matrix approach, and it is also not a natural extension of this formalism. At the same time, the extension of RSF by ρ_4 follows the (multi)particle-like state interpretation of the original RSF. Thus, when coherent pumping is omitted, it provides the simplest extension of RSF that is natural to this formalism and adds the quantum features to the description. Still, one could make analogously further extensions of RSF using three copies of single-particle space, and so on, to track higher-order correlations in photon numbers.

The important feature of the set of equations (21), (22) and (28)–(30) is that in fact they represent a finite set of first order in time differential equations. Therefore, if the time dependence of $\hat{h}, |\xi\rangle, \hat{\gamma}_\updownarrow$ is given by simple functions, one can easily find analytic solutions. Additionally, one can solve this set order by order, as solutions of tensors of lower order are independent of solutions for tensors of higher order. Simply, one solves from the lowest order, i.e. $|\alpha\rangle$ and use the solution as non-homogeneous part for the rest of equations.

The introduction of implicit linear coupling of different modes in the system Hamiltonian $\hat{H} = \sum_{k,k'} \omega_{k,k'} a_k^\dagger \hat{a}_{k'}$ is equivalent to taking a local approach in deriving the master equation where this coupling is considered to be a perturbation. Although it allows one to work explicitly with modes in desired basis, it is not always valid, and then a global approach should be considered (see [39] for a brief review). In the global approach, one first diagonalizes the system Hamiltonian and then considers the evolution of transformed modes. In the end, one transforms the obtained results by reverse unitary transformation of modes to the original basis. As described further in the text, this can be easily done on the reduced state.

Therefore, one can easily apply also global approach. In fact, the unitary transformation that diagonalizes the reduced Hamiltonian $\hat{h}$ is the same as the unitary transformation of modes that diagonalizes the original Hamiltonian. This allows for consideration of the system solely from the reduced perspective.

4.2. Local evolution

If one is interested in entanglement in a given bipartition, the structure of interest is the reduced two-particle-like state $\hat{\rho}^{\mathcal{N}}_{\rho_F}$. However, based on (28), the evolution of this matrix is, in general, not self-contained, and so the full $\hat{\rho}_4$ is required. Still, if the evolution is local in terms of a given bipartition, then the evolution of $\hat{\rho}^{\mathcal{N}}_{\rho_F}$ is closed. In this case, 'local' intuitively means that the evolution does not transfer particles between modes corresponding to two parties determined by the given bipartition or does not damp or pump them in a correlated manner. This translates to $\hat{h}$, $\hat{\gamma}_{\updownarrow}$ and all $\hat{u}_j$ being block diagonal in this bipartition, i.e. they can be written as a direct sum of matrices that act only on degrees of freedom of the given party. This allows the projector $\Pi_{\mathcal{I}_A,\mathcal{I}_B}$ to commute with tensor products of such block diagonal matrices as $\hat{h}\otimes\mathbf{1}$ in equation (28). From this, after projecting (28) into the subspace corresponding to $\Pi_{\mathcal{I}_A,\mathcal{I}_B}$, we get:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}^{\Pi}_{\rho} = &-\frac{i}{\hbar}\left[\hat{h}\otimes\mathbf{1}+\mathbf{1}\otimes\hat{h},\hat{\rho}^{\Pi}_{\rho}\right]\\ &+\Pi_{\mathcal{I}_A,\mathcal{I}_B}\left(|\xi\rangle\hat{\beta}^{\dagger}+\left(|\xi\rangle\hat{\beta}^{\dagger}\right)^{\tau_L}+\left(|\xi\rangle\langle\alpha|\otimes\mathbf{1}\right)^{\tau_L}+\hat{\beta}\langle\xi|+\left(\hat{\beta}\langle\xi|\right)^{\tau_R}+\left(\mathbf{1}\otimes|\alpha\rangle\langle\xi|\right)^{\tau_R}\right)\Pi_{\mathcal{I}_A,\mathcal{I}_B}\\ &+\sum_j\kappa_j\left(\hat{u}_j\otimes\hat{u}_j\hat{\rho}^{\Pi}_{\rho}\hat{u}_j^{\dagger}\otimes u_j^{\dagger}-\hat{\rho}^{\Pi}_{\rho}\right)+\frac{1}{2}\{(\mathbf{1}\otimes\hat{\gamma}_{\uparrow}+\hat{\gamma}_{\uparrow}\otimes\mathbf{1})-\left(\mathbf{1}\otimes\hat{\gamma}_{\downarrow}^{T}+\hat{\gamma}_{\downarrow}^{T}\otimes\mathbf{1}\right),\hat{\rho}^{\Pi}_{\rho}\}\\ &+\Pi_{\mathcal{I}_A,\mathcal{I}_B}\left[\left(\hat{\rho}\otimes\gamma_{\downarrow}^{T}\right)^{\tau_L}+\left(\gamma_{\uparrow}\otimes\hat{\rho}\right)^{\tau_L}+\gamma_{\uparrow}\otimes\hat{\rho}+\hat{\rho}\otimes\gamma_{\uparrow}+\left(\gamma_{\uparrow}\otimes\mathbf{1}\right)^{\tau_L}\right]\Pi_{\mathcal{I}_A,\mathcal{I}_B},\end{aligned}\tag{31}$$

where one simply replaces $\hat{\rho}_4\to\hat{\rho}^{\Pi}_{\rho}$ in equation (28) and projects the non-homogeneous part using $\Pi_{\mathcal{I}_A,\mathcal{I}_B}$. This allows restricting the considerations of entanglement in the extended RSF to $\hat{\rho}^{\mathcal{N}}_{\rho_F}$ instead of tracking the whole $\hat{\rho}_4$.

5. Examples: PPT criterion for multi-mode bosonic fields

We have shown that the sufficient condition for the entanglement of the full state $\hat{\rho}_F$ is that the reduced two-particle-like state $\hat{\rho}^{\mathcal{N}}_{\rho_F}$ is entangled. However, this does not mean that there exists a state $\hat{\rho}_F$ such that $\hat{\rho}^{\mathcal{N}}_{\rho_F}$ is entangled. Therefore, in the following, we show the existence of such states by presenting two examples. What is more, we show that $\hat{\rho}^{\mathcal{N}}_{\rho_F}$ contains information about the entanglement for Gaussian states and for non-Gaussian states for which the PPT criterion for the covariance matrix cannot reveal entanglement.

Because one can apply any entanglement detection method for bipartitie finite-dimensional systems to the $\hat{\rho}^{\mathcal{N}}_{\rho_F}$, let us consider one of the most widely known entanglement criteria, i.e. the PPT criterion [3]. This criterion states that it is sufficient if partial transposition of the state results in:

$$\left(\hat{\rho}^{\mathcal{N}}_{\rho_F}\right)^{T_2}<0\tag{32}$$

for state $\hat{\rho}^{\mathcal{N}}_{\rho_F}$ to be entangled. In the simplest case of a two-qubit density matrix, the PPT criterion is a sufficient and necessary condition for entanglement. Therefore, when $\hat{\rho}^{\mathcal{N}}_{\rho_F}$ is a two-qubit density matrix and the PPT criterion does not reveal the entanglement of $\hat{\rho}^{\mathcal{N}}_{\rho_F}$, then our reduced two-particle-like state is not able to reveal any entanglement of $\hat{\rho}_F$. This does not imply that the state $\hat{\rho}_F$ is necessarily a separable state. This is because the entanglement of $\hat{\rho}^{\mathcal{N}}_{\rho_F}$ is only a sufficient condition for the entanglement of $\hat{\rho}_F$. In the case of a larger number of modes, if the PPT criterion does not reveal the entanglement of $\hat{\rho}^{\mathcal{N}}_{\rho_F}$, the reduced state might still keep information about the entanglement of $\hat{\rho}_F$. However, in such a case, it has to be accessed using a different criterion. While one needs at least four modes for considerations of entanglement using $\hat{\rho}^{\mathcal{N}}_{\rho_F}$, in the following, we show a method of how one can also apply this methodology to reveal the entanglement of two-mode states.

5.1. Bright squeezed vacuum

As our first example, we will use the 2×2 bright squeezed vacuum (BSV). The non-classicality of this state was considered in stationary scenarios, including the high photon number limit [40–42], and in the context of correlation in Bose–Einstein condensates [43]. Let us consider four orthogonal modes and the bipartition given by $\mathcal{I}_A=\{1,2\}$, $\mathcal{I}_B=\{3,4\}$. The BSV state is obtained by unitary evolution of the vacuum generated by the interaction Hamiltonian [4]:

$$\hat{H}_{\text{int}}=\gamma\left(\hat{a}_1^{\dagger}\hat{a}_4^{\dagger}-\hat{a}_2^{\dagger}\hat{a}_3^{\dagger}\right)+h.c.,\tag{33}$$

and therefore it is a Gaussian state. Now, the BSV state can be written in the form:

$$|\psi_{-}\rangle = \frac{1}{\cosh^2(\Gamma)} \sum_{n=0}^{\infty} \frac{\tanh^n(\Gamma)}{n!} \left(\hat{a}_1^\dagger \hat{a}_4^\dagger - \hat{a}_2^\dagger \hat{a}_3^\dagger\right)^n |\Omega\rangle = \frac{1}{\cosh^2(\Gamma)} \sum_{n=0}^{\infty} \sqrt{n+1} \tanh^n(\Gamma) |\psi^n\rangle, \tag{34}$$

where the parameter $\Gamma = \gamma t$ denotes the amplification gain, which is related to the power of the coherent source impinged on the nonlinear crystal in the parametric down conversion process, and

$$|\psi_{-}^n\rangle = \frac{1}{\sqrt{n+1}} \sum_{m=0}^{n} (-1)^m |(n-m), m; m, (n-m)\rangle. \tag{35}$$

Calculation of $\hat{\rho}_{\psi}^{\Pi}$ yields:

$$\hat{\rho}_{\psi}^{\Pi} = \begin{pmatrix} \rho_{1313} & 0 & 0 & 0 \\ 0 & \rho_{1414} & \rho_{1423} & 0 \\ 0 & \rho_{2314} & \rho_{2323} & 0 \\ 0 & 0 & 0 & \rho_{2424} \end{pmatrix}, \tag{36}$$

where we have restricted this matrix only to the subspace determined by $\Pi_{\mathcal{I}_A,\mathcal{I}_B}$, and

$$\begin{aligned} \rho_{1313} &= \rho_{2424} = \sinh^4(\Gamma), \\ \rho_{1414} &= \rho_{2323} = \sinh^2(\Gamma)\cosh(2\Gamma), \\ \rho_{2314} &= \rho_{1423} = -\sinh^2(\Gamma)\cosh^2(\Gamma). \end{aligned} \tag{37}$$

After normalization and applying the partial transpose, we find that $(\hat{\rho}_{\psi}^{\mathcal{N}})^{T_2}$ has two eigenvalues:

$$\begin{aligned} \lambda_1 &= \frac{1}{1 - 3\cosh(2\Gamma)}, \\ \lambda_2 = \lambda_3 = \lambda_4 &= \frac{1}{3 - \operatorname{sech}(2\Gamma)}. \end{aligned} \tag{38}$$

The eigenvalue λ_1 is negative for all $\Gamma > 0$. Therefore, we applied the PPT criterion to show that the BSV state is entangled for any $\Gamma > 0$ and thus for an arbitrarily high average number of bosons. As a consequence, the two-particle space can keep information about entanglement in mesoscopic scenarios.

5.2. Single photon

A s the second example, let us also consider the state of a single photon symmetrically beam splitted into modes a_1, a_3:

$$|\Psi\rangle = \frac{1}{\sqrt{2}} (|1;0\rangle + |0;1\rangle) = \frac{1}{\sqrt{2}} \left(\hat{a}_1^\dagger + \hat{a}_3^\dagger\right) |\Omega\rangle. \tag{39}$$

This state is of particular interest as it is non-Gaussian and one cannot reveal its entanglement through the PPT criterion for the covariance matrix (see appendix A). Clearly, this is a two-mode state, and as we argued to apply the above entanglement criterion, one needs four modes. However, one can trivially extend the state to four modes by including modes a_2, a_4 with zero photons occupying these modes:

$$|\Psi\rangle = \frac{1}{\sqrt{2}} (|10;00\rangle + |00;10\rangle). \tag{40}$$

Still, this state has the form (14), for which the RSF results in $\hat{\rho}_{\Psi}^{\Pi} = \hat{0}$, and thus does not give access to information about entanglement. One can see that such a trivial extension of the two mode state will always result in $\hat{\rho}_{\rho_F}^{\Pi}$ not revealing entanglement. This is because for such an extension there can be at most one nonzero matrix element $\langle \hat{a}_1^\dagger \hat{a}_1 \hat{a}_3^\dagger \hat{a}_3 \rangle$ that is necessarily positive, and so $\hat{\rho}_{\rho_F}^{\Pi}$ in such a case is always a PPT state. Note that this can be seen as a manifestation of the fact that one is not able to observe entanglement of two-mode entangled state with simple photon counting without ancillary states acting as a reference frame.

To avoid reaching the form (14), instead of (40), one can perform a different extension of the state to four modes by, for example, introducing coherent states with real amplitude α in the additional modes:

$$|\Psi\rangle = \frac{1}{\sqrt{2}} (|1\alpha;0\alpha\rangle + |0\alpha;1\alpha\rangle) = \frac{e^{-\alpha^2}}{\sqrt{2}} \left(\hat{a}_1^\dagger + \hat{a}_3^\dagger\right) \left(\sum_{n=0}^{\infty} \frac{\alpha^n \hat{a}_2^\dagger}{\sqrt{n!}}\right) \left(\sum_{m=0}^{\infty} \frac{\alpha^m \hat{a}_4^\dagger}{\sqrt{m!}}\right) |\Omega\rangle. \tag{41}$$

This extension resembles performing a homodyne measurement on the single-photon state. However, for example, the assumption of matching energy was not done at this step, which would be required to perform the necessary interferometry for homodyne measurement. This is also not fully equivalent to performing homodyne measurement as one is interested in measuring the number of photons instead of quadratures. Such schemes are sometimes referred to as weak homodyne measurement [44–46]. Now, using the same partition $\mathcal{I}_A = \{1,2\}, \mathcal{I}_B = \{3,4\}$, we get the following normalized reduced state $\hat{\rho}^{\mathcal{N}}_{\Psi}$:

$$\hat{\rho}^{\mathcal{N}}_{\Psi} = \frac{1}{\alpha^2+\alpha^4}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{\alpha^2}{2} & \frac{\alpha^2}{2} & 0 \\ 0 & \frac{\alpha^2}{2} & \frac{\alpha^2}{2} & 0 \\ 0 & 0 & 0 & \alpha^4 \end{pmatrix}. \tag{42}$$

After partial transposition, there are three eigenvalues of the resulting matrix:

$$\begin{aligned} \lambda_1 &= \frac{\alpha^2 - \sqrt{\alpha^4+1}}{2(\alpha^2+1)}, \\ \lambda_2 &= \frac{\alpha^2 + \sqrt{\alpha^4+1}}{2(\alpha^2+1)}, \\ \lambda_3 = \lambda_4 &= \frac{1}{2(\alpha^2+1)}, \end{aligned} \tag{43}$$

where the first eigenvalue is negative for any finite $\alpha > 0$. Therefore, even for two-mode entangled states, one can retrieve information about entanglement from the extended RSF. Note that the lowest value of λ_1 is obtained for $\alpha = 0$. This is because one needs $\alpha \neq 0$ to allow normalization of the matrix, yet coherent states do not add entanglement to the system but rather some form of noise. Thus, optimally, one should have $\alpha \ll 1$ in this scenario.

5.3. Time evolution of entanglement

Let us apply the rest of the extended RSF toolbox to consider how entanglement behaves under non-unitary evolution resulting from decoherence coming from the environment. We first consider that one distributes a single-photon state $|\Psi\rangle$ between two distant parties that want to perform a weak homodyne measurement locally to reveal the entanglement of the state. This is an interesting example because a device-independent quantum key distribution protocol can be constructed based on such a setup [47], and maintaining entanglement during transmission is necessary for its success. However, the state during transmission of the photon necessarily undergoes decoherence. Let us assume that during the distribution of the state, the transmission line is affected by the thermal environment with temperature T, while the local oscillators (coherent states) are approximately not affected. In this scenario, the operators $\hat{\gamma}_{\updownarrow}$ are diagonal and fulfill the relation: $\hat{\gamma}_{\uparrow} = \mathrm{e}^{-\hbar\omega/k_bT}\hat{\gamma}_{\downarrow}$, where ω stands for the angular frequency of the modes, and k_b is Boltzmann constant. The creation rates are given by:

$$\Gamma^{kk}_{\uparrow} = \gamma_\omega N(\omega)\left(\delta_{k1} + \delta_{k3}\right), \tag{44}$$

where δ_{nm} stands for Kronecker delta, and coefficient γ_ω determines the coupling of the bath to modes with frequency ω, and $N(\omega) = 1/(\mathrm{e}^{\hbar\omega/k_bT} - 1)$ is Planck distribution of the average number of photons in the bath [48]. Furthermore, as all modes are separated up to the moment of the measurement, there is also no coupling between modes. Consequently, the Hamiltonian is simply a free Hamiltonian for four modes with the same frequency. Based on our discussion in section 4.2, for this scenario, we can consider only the evolution of reduced single- and two-particle states: $\hat{\rho}$, $\hat{\rho}^{\Pi}_{\rho_\Psi}$. Due to the trivial free evolution Hamiltonian, the master equation simplifies to:

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho} = \frac{1}{2}\{\hat{\gamma}_{\uparrow} - \hat{\gamma}_{\downarrow}^T, \hat{\rho}\} + \hat{\gamma}_{\uparrow}, \tag{45}$$

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}^{\Pi}_{\Psi} &= \frac{1}{2}\{(\mathbf{1}\otimes\hat{\gamma}_{\uparrow} + \hat{\gamma}_{\uparrow}\otimes\mathbf{1}) - \left(\mathbf{1}\otimes\hat{\gamma}_{\downarrow}^T + \hat{\gamma}_{\downarrow}^T\otimes\mathbf{1}\right), \hat{\rho}^{\Pi}_{\Psi}\} \\ &\quad + \Pi_{\mathcal{I}_A,\mathcal{I}_B}, \left(\left(\hat{\rho}\otimes\gamma_{\downarrow}^T\right)^{\mathcal{T}_L} + (\gamma_{\uparrow}\otimes\hat{\rho})^{\mathcal{T}_L} + \gamma_{\uparrow}\otimes\hat{\rho} + \hat{\rho}\otimes\gamma_{\uparrow} + (\gamma_{\uparrow}\otimes\mathbf{1})^{\mathcal{T}_L}\right)\Pi_{\mathcal{I}_A,\mathcal{I}_B}. \end{aligned} \tag{46}$$

Using initial condition for the reduced state $\hat{\rho}$:

$$\hat{\rho}(0) = \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & \alpha^2 & 0 & \alpha^2 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & \alpha^2 & 0 & \alpha^2 \end{pmatrix}, \tag{47}$$

we obtain the following time evolution of the $\hat{\rho}^{\Pi}_{\Psi}$:

$$\hat{\rho}^{\Pi}_{\Psi}(t) = \begin{pmatrix} e^{-2\gamma_\omega t}\lambda(\lambda+1) & 0 & 0 & 0 \\ 0 & \frac{1}{2}\alpha^2 e^{-\gamma_\omega t}(2\lambda+1) & \frac{1}{2}\alpha^2 e^{-\gamma_\omega t} & 0 \\ 0 & \frac{1}{2}\alpha^2 e^{-\gamma_\omega t} & \frac{1}{2}\alpha^2 e^{-\gamma_\omega t}(2\lambda+1) & 0 \\ 0 & 0 & 0 & \alpha^4 \end{pmatrix}, \tag{48}$$

where $\lambda = N(\omega)(e^{\gamma_\omega t} - 1)$. Now, in order to access information about entanglement, we apply the PPT criterion after normalization. In the result, we find that there is again one eigenvalue that can be negative:

$$\lambda_-(t) = \frac{1}{2\mathcal{N}}\left[\alpha^4 + \lambda e^{-2t\gamma_\omega}(\lambda+1) - e^{-5t\gamma_\omega}\sqrt{e^{6t\gamma_\omega}\left(\alpha^8 e^{4t\gamma_\omega} - \alpha^4 e^{2t\gamma_\omega}(2\lambda(\lambda+1)-1) + \lambda^2(\lambda+1)^2\right)}\right], \tag{49}$$

where $\mathcal{N}$ stands for the normalization factor of $\hat{\rho}^{\Pi}_{\Psi}(t)$.

Let us first consider $\lambda_-(t)$ in the limit $t \to \infty$. In this case, there are two options:

$$\lim_{t\to\infty} \lambda_-(t) = N(\omega)^2 / \left(\alpha^2 + N(\omega)\right)^2 \quad \text{for } \alpha^2 \geqslant N(\omega), \tag{50}$$

$$\lim_{t\to\infty} \lambda_-(t) = \alpha^4 / \left(\alpha^2 + N(\omega)\right)^2 \quad \text{for } \alpha^2 < N(\omega). \tag{51}$$

Remarkably, if $\alpha \neq 0$ and the bath temperature is $T = 0$ ($N(\omega) = 0$) in this limit, one has $\lambda_-(t) = 0$, which suggests that the extended RSF formalism finds the state entangled for any finite time t. To see that this is the case, first note that:

$$\lim_{N(\omega)\to 0} \lambda_-(t) = \frac{\alpha^4 - \sqrt{\alpha^8 + \alpha^4 e^{-2t\gamma_\omega}}}{2\mathcal{N}}. \tag{52}$$

Clearly, the second term of the nominator has a higher absolute value, as it is a decreasing function of time with the limit $t \to \infty$ equal to α^4. Therefore, the second term determines the sign of the nominator to be negative. Because the denominator is always positive (as it is the sum of expectation values containing only photon number operators that are non-negative), we find that $\lambda_-(t)$ is also negative in this case for any finite t. This certifies the entanglement of the state in the whole time range. Still, for any $T > 0$, the limit of $\lambda_-(t)$ as $t \to \infty$ is positive, and therefore at some finite time the entanglement will no longer be seen within the RSF formalism. Let us stress that this does not have to imply that the state is no longer entangled, as RSF provides only a sufficient criterion. This indicates that there is no detectable entanglement of the particular kind considered by RSF, i.e. photon number entanglement based on linear correlations. Solving $\lambda_-(t) = 0$ for t, one finds that this criterion does not detect entanglement after the critical time t_c:

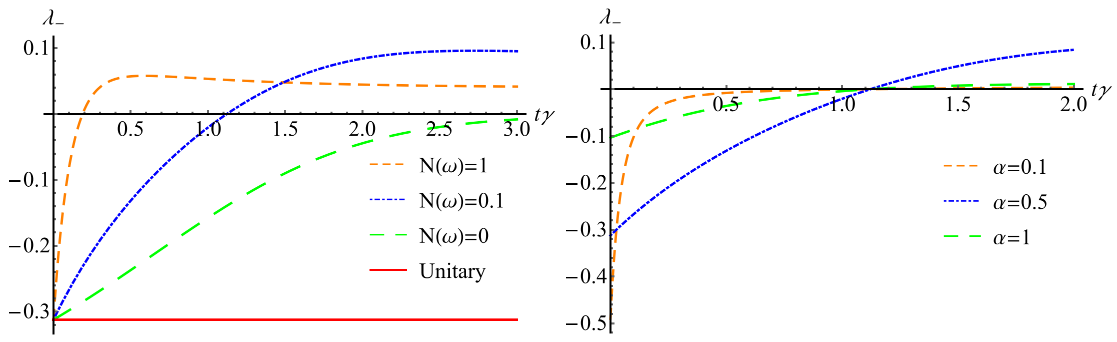
$$t_c\gamma_\omega = \log\left(1 + \frac{\sqrt{2}-1}{2N(\omega)}\right), \tag{53}$$

which clearly goes to infinity for $N(\omega) \to 0$ and to 0 for $N(\omega) \to \infty$. Interestingly, t_c is independent of α and therefore α only affects the magnitude of $\lambda_-(t)$ and not its qualitative behavior in terms of its sign.

Let us comment that, in general, extensions of the state do not have to be equivalent. For example, one can try to engineer an optimal ancilla to maximally violate some Bell inequality [49]. Here, we also see this kind of inequivalence, since the different extensions (by different coherent states) give different magnitudes of $\lambda_-(t)$. In addition, one can have a completely different behavior, as found, for example, with the trivial extension considered before. Therefore, it is interesting to see that different non-trivial extensions result in the same t_c. However, it is not a general property of all non-trivial extensions. Assuming only that the extended part of the state is separable from the original state, one can find for the considered single-photon state that:

$$\hat{\rho}^{\Pi}_{\Psi} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{\langle \hat{a}_4^\dagger \hat{a}_4 \rangle}{2} & \frac{\langle \hat{a}_2^\dagger \hat{a}_4 \rangle}{2} & 0 \\ 0 & \frac{\langle \hat{a}_4^\dagger \hat{a}_2 \rangle}{2} & \frac{\langle \hat{a}_2^\dagger \hat{a}_2 \rangle}{2} & 0 \\ 0 & 0 & 0 & \langle \hat{a}_2^\dagger \hat{a}_2 \hat{a}_4^\dagger \hat{a}_4 \rangle \end{pmatrix}. \tag{54}$$

From this, one can see that any extension for which $\langle \hat{a}_2^\dagger \hat{a}_4 \rangle = 0$ will not find entanglement. Thus, in this scenario, one excludes any Fock states as meaningful extensions. Performing calculations analogous to (53), one finds:



(a) (b)

Figure 1. (a) Time evolution of $\lambda_-(t)$ for $\alpha = 0.5$ and different values of $N(\omega)$. The solid red line presents the value of $\lambda_-(t)$ in the case of unitary evolution without a thermal environment. For $N(\omega) = 0$ value of $\lambda_-(t)$ converges to zero but is always negative, showing the entanglement of the state. With increasing $N(\omega)$ the photon number entanglement starts to decay faster, eventually disappearing. (b) Time evolution of $\lambda_-(t)$ for $N(\omega) = 0.1$ and different values of α. For all values of α axis is reached at the same time t_c. The value of $\lambda_-(0)$ increases with α. However, the rate of growth of α greatly decreases for higher values of α. This can be seen as the curve for $\alpha = 0.1$ quickly crosses other curves while still being negative, and therefore extremely small values of α are no longer optimal as in the unitary case.

$$t_c\gamma_\omega = \log\left(1 + \frac{\sqrt{1 + |\langle \hat{a}_2^\dagger \hat{a}_4\rangle|^2/\langle \hat{a}_2^\dagger \hat{a}_2 \hat{a}_4^\dagger \hat{a}_4\rangle} - 1}{2N(\omega)}\right), \tag{55}$$

which clearly depends on the form of the extension. Then, for the single-photon state (39), the optimal extensions are the ones that maximize $|\langle \hat{a}_2^\dagger \hat{a}_4\rangle|^2/\langle \hat{a}_2^\dagger \hat{a}_2 \hat{a}_4^\dagger \hat{a}_4\rangle$. If the ancillary state is a separable state, then by the Cauchy-Schwarz inequality, one can find that this quantity is bounded by 1 [50]. Thus, since the extension by coherent states saturates this bound, it gives an optimal value of t_c. Figure 1 presents examples of the evolution of the eigenvalue $\lambda_-(t)$ in different regimes. Clearly, entanglement becomes weaker with time evolution, and its decay becomes faster with increasing $N(\omega)$. In general, this shows that the single-photon entangled state is a resource that is quite robust against thermal damping when the thermal bath has a low temperature.

Let us note that one can propose one extension which is not built from a separable state. In particular, a second copy of the original state can be taken as such an extension. This still indicates that the observed entanglement is due to the entanglement of the original state. However, in such a case, it is rather sensible that the ancillary modes undergo the same evolution as the modes of the original state. This is because the state of the ancillary modes cannot be prepared locally. Thus, for the considered scenario, one should take the following creation rates:

$$\Gamma_\uparrow^{kk} = \gamma_\omega N(\omega)\,\delta_{kk}. \tag{56}$$

For this case, t_c is exactly the same as for the case of the extension by coherent states. Thus, this simple extension by the second copy of the state is also optimal in this case.

Now, let us consider an analogous scenario for the BSV state where all modes are coupled to the thermal environment with the same temperature during the distribution of the state between parties. Therefore, for this case, we consider the creation rates (56). Then, using as initial conditions reduced states (36) and

$$\rho = \mathrm{diag}\left(\sinh^2(\Gamma), \sinh^2(\Gamma), \sinh^2(\Gamma), \sinh^2(\Gamma)\right), \tag{57}$$

we get the following solution for $\hat{\rho}_\psi^\Pi$:

$$\hat{\rho}_\psi^\Pi(t) = \begin{pmatrix} \rho_{1313}(t) & 0 & 0 & 0 \\ 0 & \rho_{1414}(t) & \rho_{1423}(t) & 0 \\ 0 & \rho_{2314}(t) & \rho_{2323}(t) & 0 \\ 0 & 0 & 0 & \rho_{2424}(t) \end{pmatrix}, \tag{58}$$

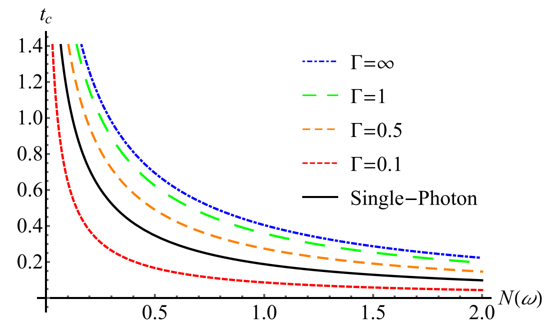


Figure 2. Comparison of t_c for the single-photon state and the BSV state for different Γ as a function of $N(\omega)$. The critical time t_c for the BSV state quickly converges to the limiting case $\Gamma \to \infty$ and reaches a significant advantage in robustness over the single-photon state. Still, for small values of Γ, entanglement of the single-photon state is more robust against non-unitary evolution resulting from thermal bath.

where

$$\begin{aligned} \rho_{1313} &= \rho_{2424} = \frac{1}{4} e^{-2\gamma_\omega t} \left(\cosh(2\Gamma) + 2\lambda - 1\right)^2, \\ \rho_{1414} &= \rho_{2323} = e^{-2\gamma_\omega t} \left(\cosh(2\Gamma)\left(\sinh^2(\Gamma) + \lambda\right) + (\lambda - 1)\lambda\right), \\ \rho_{2314} &= \rho_{1423} = -e^{-2\gamma_\omega t} \sinh^2(\Gamma)\cosh^2(\Gamma). \end{aligned} \tag{59}$$

Applying the PPT criterion, we find that the negative eigenvalue evolves as follows:

$$\lambda_1(t) = \frac{1}{4} - \frac{3\sinh^2(2\Gamma)}{2\left(8(2\lambda - 1)\cosh(2\Gamma) + 3\cosh(4\Gamma) + 16(\lambda - 1)\lambda + 5\right)}. \tag{60}$$

With the realization that the only time dependence is in λ, which for the special case of $T = 0$ is equal to 0, one can see that the entanglement of the BSV state is, in fact, completely stationary under the considered non-unitary evolution, i.e.

$$\lambda_1(t) = \lambda_1(0). \tag{61}$$

This shows the exceptional robustness of the BSV state to low-temperature damping. For any non-zero temperature ($T \neq 0$), there is a point in time at which the entanglement is not detected any more:

$$t_c\gamma_\omega = \log\left(1 + \frac{e^{-\Gamma}\sinh(\Gamma)}{N(\omega)}\right), \tag{62}$$

and for $t \to \infty$ the eigenvalue $\lambda_1(t)$ converges to $1/4$. Note that t_c is an increasing function of the pumping parameter with the limit

$$\lim_{\Gamma\to\infty} t_c\gamma_\omega = \log\left(1 + \frac{1}{2N(\omega)}\right). \tag{63}$$

Compering this expression to critical time for the single-photon state (53), one can see that the critical time for the highly pumped BSV state is more robust against this type of decoherence. Still, for small values of Γ where the BSV state is dominated by the vacuum component, t_c can be smaller than for the single-photon state. This happens for $\Gamma < -\log(2 - \sqrt{2})/2 \approx 0.27$. Figure 2 shows comparison of t_c for BSV state with different values of Γ and single-photon state.

5.4. Relation with covariance matrix for Gaussian states

Let us stress that detection of entanglement in a case of some Gaussian states does not imply that $\hat{\rho}^{\mathcal{N}}_{\rho_F}$ can reveal entanglement for any entangled Gaussian state. The reason for this is that while the covariance matrix keeps full information about the Gaussian state, our $\hat{\rho}^{\mathcal{N}}_{\rho_F}$ stores information only about a particular type of correlations.

The general inequivalence of these criteria for Gaussian states can be seen based on the two-mode squeezed vacuum state. As we discussed earlier, for the trivial extension of the two-mode state, one is unable to find the entanglement in terms of $\hat{\rho}^{\mathcal{N}}_{\rho_F}$, and the proper extension has to be chosen. At the same time, the PPT criterion for the covariance matrix finds that the state is entangled. However, choosing a suitable extension will allow the entanglement of the considered state to be found using $\hat{\rho}^{\mathcal{N}}_{\rho_F}$. As in the case of the single-photon state, one can take a second copy of the state as an extension to find the entanglement. Then, the extended state is, in fact, analogous to the BSV state (with the difference that the two ancillary modes are phase-shifted in total by π), for which $\hat{\rho}^{\mathcal{N}}_{\rho_F}$ keeps information about entanglement. To see this, note that the Hamiltonian that generates the BSV state (33) consists of two commuting parts $\hat{H}_{14}$ and $\hat{H}_{23}$ acting on different sets of modes: $\{a_1, a_4\}$ and $\{a_2, a_3\}$. Thus, the unitary evolution of the modes under this Hamiltonian factorizes as $\mathrm{e}^{-i\hat{H}_{14}t/\hbar}\mathrm{e}^{-i\hat{H}_{23}t/\hbar}$ where each exponent corresponds to two-mode squeezing. From this it is apparent that this evolution with the vacuum as the initial state creates a product of two two-mode squeezed vacuum states. However, squeezing parameters for these pairs of modes have the opposite sign based on (33).

Observe also that entanglement in Gaussian states is created only through squeezing. In particular, two-mode squeezing creates correlated particle pairs. Therefore, since this type of correlation is in the core of $\hat{\rho}^{\mathcal{N}}_{\rho_F}$, it should be efficient in detecting the entanglement of Gaussian states. Moreover, entanglement from single-mode squeezing appears by beam splitting or, more generally speaking, by linear couplings with other modes. From our discussion, we saw that the entanglement created by the beam splitting can be captured by $\hat{\rho}^{\mathcal{N}}_{\rho_F}$, and thus is similar in nature. Consider, as an example, a specific class of entangled Gaussian states. In particular, assume that one starts with the state resulting from some squeezing of different pairs of modes. Then, allow the full state of these modes to evolve based on some Hamiltonian that admits the RSF reduction and couples only modes local to a given party. Before time evolution, one should be able to find if such a state is entangled using $\hat{\rho}^{\mathcal{N}}_{\rho_F}$ based on our disscusion (this may require taking a copy of the state as the extension). Now, the evolution equation (31) in our scenario is simply a Heisenberg equation. It generates a unitary evolution that factorizes with respect to subsystems: $\mathrm{e}^{-i\hat{h}_A t/\hbar}\otimes\mathrm{e}^{-i\hat{h}_B t/\hbar}$, where $\hat{h}_{A(B)}$ is a reduced Hamiltonian restricted to the modes of subsystem A (B). Now, one can write $\hat{\rho}^{\mathcal{N}}_{\rho_F}$ in the product basis that diagonalizes $\hat{h}_A$ and $\hat{h}_B$. Importantly, the choice of the particular local basis does not affect whether the PPT criterion finds entanglement. Then, one is left with local free evolution that does not destroy entanglement in the given bipartition. Thus, $\hat{\rho}^{\mathcal{N}}_{\rho_F}$ detects entanglement for the considered class of Gaussian states.

5.5. Maximally mixed states

Let us consider the limit $t\to\infty$ of the reduced two-particle-like state $\hat{\rho}^{\Pi}_{\psi}(t)$ in (58). In this limit, one gets:

$$\lim_{t\to\infty}\hat{\rho}^{\Pi}_{\psi}(t) = \mathrm{diag}\left(N(\omega)^2, N(\omega)^2, N(\omega)^2, N(\omega)^2\right). \tag{64}$$

After normalization, this matrix corresponds to the maximally mixed state on the subspace of the two-particle space restricted to the given bipartition. As the bath in this example was thermal and the same for all modes, this reduced two-particle-like state corresponds to the four-mode thermal state for a given temperature T. Note that the temperature does not affect the normalized reduced state. Similarly, for this state, we have $\hat{\rho} = \mathrm{diag}(N(\omega), N(\omega), N(\omega), N(\omega))$, which constitutes a maximally mixed state in a single-particle space. As the inclusion of additional separable modes in the thermal state for a given T cannot add any new type of correlations seen in the reduced states, one can see that the thermal states always correspond to maximally mixed states on single and two particle spaces.

6. Passive optical elements

Most optical devices include passive optical elements, such as beam splitters and phase shifters. The RSF formalism allows for easy introduction of such elements into the system. Therefore, this formalism allows for a straightforward analysis of experimental setups. Let us start with the phase shifter. We assume that the beam contains the mode a_i at some point in time, starts the interaction with the phase shifter at $t=\tau_0$ and ends it at $t=\tau_e$, which adds the phase to this particular mode. This can be achieved by the following modification of the Hamiltonian:

$$\hat{H}\to\hat{H}+\phi_i I_{[\tau_0,\tau_e]}(t)\,\hat{a}_i^{\dagger}\hat{a}_i, \tag{65}$$

where $I_{[\tau_0,\tau_e]}(t)$ stands for the indicator function on the time interval $[\tau_0,\tau_e]$, and ϕ_i determines the phase gain rate of ith mode. The resulting final phase shift is given by:

$$\Delta\phi = (\tau_e-\tau_0)\,\phi_i. \tag{66}$$

The beam splitting of two modes a_i, a_j into two modes a_i', a_j' can be effectively realized as a unitary transformation of the corresponding annihilation and creation operators given by:

$$\begin{pmatrix} \hat{a}_i' \\ \hat{a}_j' \end{pmatrix} = \begin{pmatrix} \sqrt{T} & i\sqrt{R} \\ i\sqrt{R} & \sqrt{T} \end{pmatrix} \begin{pmatrix} \hat{a}_i \\ \hat{a}_j \end{pmatrix} = \mathbf{U}_T \begin{pmatrix} \hat{a}_i \\ \hat{a}_j \end{pmatrix}, \tag{67}$$

where R and T stand for reflectivity and transmissivity, respectively. Before beam splitting, modes a_i', a_j' are in the ground state, and after this transformation, modes a_i, a_j are left empty. Therefore, their roles interchange, and tracking modes a_i, a_j is of no use after the operation. Therefore, just after the operation, one can rename the modes a_i', a_j' to a_i, a_j, keeping the structure of the reduced state. Based on equation (17), one can find that any unitary transformation $\mathbf{U}$ of annihilation operators reduces to the operator:

$$\mathbf{U} \to \hat{u} = \sum_{i,j} U_{ji} |j\rangle\langle i|, \tag{68}$$

where U_{ji} stand for matrix elements of $\mathbf{U}$. Then, under beam splitting operation, the full reduced state transforms as follows:

$$\begin{aligned} \hat{\rho}_4 &\to \hat{u}_T \otimes \hat{u}_T \hat{\rho}_4 \hat{u}_T^\dagger \otimes \hat{u}_T^\dagger, \\ \hat{\beta} &\to \hat{u}_T \otimes \hat{u}_T \hat{\beta} \hat{u}_T^\dagger, \\ \hat{\rho} &\to \hat{u}_T \hat{\rho} \hat{u}_T^\dagger, \\ \hat{r} &\to \hat{u}_T \hat{r} \hat{u}_T^T, \\ |\alpha\rangle &\to \hat{u}_T |\alpha\rangle. \end{aligned} \tag{69}$$

Note that one can analogously incorporate to the analysis phase shifting in an instantaneous manner as it results in unitary mode transformation. This reduction of unitary transformations of modes also allows one to consider the inefficiency of the detectors, which can be modeled as a two-port beamsplitter on the path of the mode a_i with transmissivity equal to efficiency $T = \eta$ and second output mode traced out. Denoting the efficiency of the detector at mode a_i as η_i, inefficient detectors can be applied by operation:

$$\hat{\eta} = \sum_i \sqrt{\eta_i} |i\rangle\langle i|. \tag{70}$$

Then, the reduced state $\hat{\rho}$ transforms as $\hat{\rho} \to \hat{\eta}\rho\hat{\eta}$, and other parts of the reduced state transform analogously.

Assuming equal efficiency η of all detectors, one can see that entanglement of the BSV state can be revealed for arbitrary efficiency, as the matrix $\hat{\rho}_\psi^\Pi$ (36) is varied only by constant coefficient η^2, which is removed after normalization. Thus, after partial transposition, the eigenvalues are not changed. In fact, this applies to any state and any entanglement criterion by the same means.

Let us go back to the unitary transformation $\mathbf{U}_d$ of the modes that diagonalize the original Hamiltonian $\hat{H}$. Clearly, the diagonalized Hamiltonian $\hat{H}_d$ reduces to the diagonal Hamiltonian $\hat{h}_d$. As the unitary transformation of modes reduces by (68), one gets:

$$\hat{u}_d \hat{h} \hat{u}_d^\dagger = \hat{h}_d, \tag{71}$$

where the equality stands for equality of the matrices representing operators in specific basis in which h_d is diagonal. Therefore, the reduced operators $\hat{u}_d$ perform the diagonalization of the reduced Hamiltonian. On the other hand, if one finds a unitary operator $\hat{u}_d$ that fulfills (71) for some $\hat{h}_d$, because the reduction of the Hamiltonian is a bijection, one knows that there is a corresponding diagonal Hamiltonian in the Fock space $\hat{H}_d$ that must be obtained by mode transformation from the original Hamiltonian $\hat{H}$. However, since the reduction of unitary transformations of modes is also bijective, this transformation is obtained from $\hat{u}_d$.

6.1. Homodyne measurement and squeezed states pumping

One of the tools used in quantum optics is homodyne measurements. In such measurements on state $\hat{\rho}_F$, one interferes the coherent state through beamsplitter with state $\hat{\rho}_F$ and performs intensity measurement or photon counting. Such schemes can be analyzed in the RSF formalism as it requires only extending the reduced state by modes in coherent states (see the appendix B) and performing a beam splitting operation on the obtained reduced state. However, as presented above, in some circumstances one does not even have to mathematically perform a beam splitting operation to get access to information about entanglement.

One of the drawbacks of the RSF formalism is the absence of the possibility of direct inclusion of the squeezing in the evolution of the system. However, there is a partial solution to this problem. In many experimental setups, first some modes are impulsed pumped with squeezed states coming, for example, from parametric down conversion and then combined with the rest of the system through beamsplitters. As one can easily calculate the reduced state for the squeezed states, analogously to the case of homodyne measurements, one can combine the modes in squeezed states with the reduced state of the system. Therefore, one can effectively include some form of squeezing in the system. What is more, one can also include in such a way higher-order squeezed states [5].

7. Mandel-Q parameter and two mode entanglement

Our extension of RSF is not limited only to revealing entanglement in terms of non-classical phenomena. One of the non-classical phenomena in quantum optics is the sub-Poissonian photon statistics of light, which has no classical counterpart. To quantify this phenomenon, one can use the Mandel Q parameter [51]:

$$Q_i = \frac{\langle \hat{a}_i^\dagger \hat{a}_i \hat{a}_i^\dagger \hat{a}_i \rangle - \langle \hat{a}_i^\dagger \hat{a}_i \rangle^2}{\langle \hat{a}_i^\dagger \hat{a}_i \rangle} - 1. \tag{72}$$

If $Q_i < 0$, the state of the mode a_i has sub-Poissonian statistics. This non-classical behavior is still widely studied and used, for example, for source verification [52–54], in particular, using the time-dependent version of this parameter. Clearly, the extended RSF formalism keeps information on photon statistics and its time dependence in the operators $\hat{\rho}(t), \hat{\rho}_4(t)$ and so the Mandel Q parameter can be found as:

$$Q_i = \frac{\mathrm{tr}\left\{|i,i\rangle\langle i,i|\left(\hat{\rho}_4 - \hat{\rho}\otimes\hat{\rho}\right)\right\}}{\mathrm{tr}\left\{|i\rangle\langle i|\hat{\rho}\right\}} - 1. \tag{73}$$

This is one of the reasons why one would want to include $\hat{\rho}_4$ in the extension of RSF instead of only $\hat{\rho}^{\Pi}$. The Mandel Q parameter, which is a shifted and rescaled variance, allows for detecting non-classical behavior internal to the state of a single mode. Still, other parts of the covariance matrix (note that this is a different covariance matrix from the previously mentioned covariance matrix associated with quadratures) that mixes two modes a_i, a_j can also be used to reveal non-classicality, which is shared among multiple modes. Let us build a generalization of the Mandel Q parameter using the criterion for the two-mode entanglement from [50]:

$$\langle \hat{a}_i^\dagger \hat{a}_i \hat{a}_j^\dagger \hat{a}_j \rangle - \langle \hat{a}_i^\dagger \hat{a}_j \rangle \langle \hat{a}_j^\dagger \hat{a}_i \rangle < 0 \implies \mathcal{Q}_{ij} \equiv \frac{\langle \hat{a}_i^\dagger \hat{a}_j \hat{a}_j^\dagger \hat{a}_i \rangle - \langle \hat{a}_i^\dagger \hat{a}_j \rangle \langle \hat{a}_j^\dagger \hat{a}_i \rangle}{\langle \hat{a}_i^\dagger \hat{a}_i \rangle} - 1 < 0, \tag{74}$$

where we have used commutation relation $[\hat{a}_j, \hat{a}_j^\dagger] = 1$ and the fact that $\langle \hat{a}_i^\dagger \hat{a}_i \rangle$ is non negative. In fact, this parameter contains the covariance of the operators $\hat{a}_j^\dagger \hat{a}_i$, $\hat{a}_i^\dagger \hat{a}_j$, and clearly it highly resembles the Mandel Q parameter as $\mathcal{Q}_{ii} = Q_i$. In terms of RSF, one can calculate the parameter $\mathcal{Q}_{ij}$ as:

$$\mathcal{Q}_{ij} = \frac{\mathrm{tr}\left\{|j,i\rangle\langle i,j|\left(\hat{\rho}_4 - \hat{\rho}\otimes\hat{\rho}\right)\right\}}{\mathrm{tr}\left\{|i\rangle\langle i|\hat{\rho}\right\}} - 1. \tag{75}$$

For the maximally entangled state of a single photon shared among two modes (39), one gets $\mathcal{Q}_{13} = \mathcal{Q}_{31} = 1/2$. For this state, the time evolution analogous to the one considered in previous sections leads to:

$$\mathcal{Q}_{13} = \mathcal{Q}_{31} = \frac{\left(4\lambda\left(\lambda+1\right)-1\right)\mathrm{e}^{-2\gamma_\omega t}}{\mathrm{e}^{-\gamma_\omega t}\left(\frac{1}{2} - N(\omega)\right) + N(\omega)}. \tag{76}$$

One can find that $\mathcal{Q}_{13} = 0$ at exactly the same time t_c as the scenario with ancillary coherent states (53). For $\mathcal{Q}_{13}$, adding ancillary states to reveal the entanglement turned out to be unnecessary as this parameter uses additional information contained in $\hat{\rho}$.

Let us also remark some additional similarities of $\mathcal{Q}_{ij}$ with Q_i. Consider $\mathcal{Q}_{12}$ for a two-mode coherent state in modes a_1, a_2 with complex amplitudes α_1, α_2. In this scenario, one can find that:

$$\mathcal{Q}_{12} = \frac{|\alpha_1|^2|\alpha_2|^2 + |\alpha_1|^2 - |\alpha_1|^2|\alpha_2|^2}{|\alpha_1|^2} - 1 = 0. \tag{77}$$

Let us recall that whenever $Q_i = 0$, the photon counting in the mode i is a Poissonian process, which is always the case for the coherent states. Now, consider a two-mode thermal state:

$$\hat{\rho}_{\mathrm{th}} = \sum_{i=0}^{\infty} \frac{N_1(\omega)^i}{\left(N_1(\omega)+1\right)^{i+1}} \sum_{j=0}^{\infty} \frac{N_2(\omega)^j}{\left(N_2(\omega)+1\right)^{j+1}} |i;j\rangle\langle i;j|, \tag{78}$$

where $N_q(\omega)$ is the average number of photons in mode q. For this state, one gets:

$$\mathcal{Q}_{ij} = N_j(\omega). \tag{79}$$

Note that for the thermal state, the Mandel Q parameter has the same value $Q_j = N_j(\omega)$ that exceeds corresponding value in the Poissonian case. One can observe the high resemblance between the values of $\mathcal{Q}_{ij}$ and $\mathcal{Q}_{ii}$, suggesting a deeper connection between these two.

7.1. Transformation of sub-Poissonian statistics into two mode entanglement

Consider two mode state $\hat{\rho}_\Phi$ with one of the modes in an arbitrarily state $\hat{\rho}_\varphi$ and the second one in the zero photon state:

$$\hat{\rho}_\Phi = \hat{\rho}_\varphi \otimes |0\rangle\langle 0|. \tag{80}$$

The relevant reduced states for parameter $\mathcal{Q}_{ij}$ are the following:

$$\hat{\rho} = \begin{pmatrix} \langle \hat{n}_1 \rangle & 0 \\ 0 & 0 \end{pmatrix}, \quad \hat{\rho}_4 = \begin{pmatrix} \langle \hat{n}_1^2 \rangle & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & \langle \hat{n}_1 \rangle & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{81}$$

Let us now consider a scenario in which one performs the beam splitting operation on this state. Applying beam splitting transformation (69) to the reduced states (81), one can calculate parameter $\mathcal{Q}_{ij}^{\text{out}}$ for the output modes:

$$\mathcal{Q}_{12}^{\text{out}} = \frac{\langle \hat{n}_1^2 \rangle RT + \langle \hat{n}_1 \rangle T^2 - \langle \hat{n}_1 \rangle^2 RT}{\langle \hat{n}_1 \rangle T} - 1, \tag{82}$$

$$\mathcal{Q}_{21}^{\text{out}} = \frac{\langle \hat{n}_1^2 \rangle RT + \langle \hat{n}_1 \rangle R^2 - \langle \hat{n}_1 \rangle^2 RT}{\langle \hat{n}_1 \rangle R} - 1, \tag{83}$$

$$\mathcal{Q}_{11}^{\text{out}} = \frac{\langle \hat{n}_1^2 \rangle T^2 + \langle \hat{n}_1 \rangle RT - \langle \hat{n}_1 \rangle^2 T^2}{\langle \hat{n}_1 \rangle T} - 1, \tag{84}$$

$$\mathcal{Q}_{22}^{\text{out}} = \frac{\langle \hat{n}_1^2 \rangle R^2 + \langle \hat{n}_1 \rangle RT - \langle \hat{n}_1 \rangle^2 R^2}{\langle \hat{n}_1 \rangle R} - 1. \tag{85}$$

Note that $\mathcal{Q}_{21}^{\text{out}} + \mathcal{Q}_{12}^{\text{out}} = \mathcal{Q}_{22}^{\text{out}} + \mathcal{Q}_{11}^{\text{out}}$, and so entangled state resulting from the beam splitting has at least one of the modes necessarily sub-Poissonian locally. In fact, both of them have to be sub-Poissonian as:

$$\mathcal{Q}_{11}^{\text{out}} = T\frac{\langle \hat{n}_1^2 \rangle - \langle \hat{n}_1 \rangle^2}{\langle \hat{n}_1 \rangle} + R - 1 = T\frac{\langle \hat{n}_1^2 \rangle - \langle \hat{n}_1 \rangle^2}{\langle \hat{n}_1 \rangle} - T = T\mathcal{Q}_{11}^{\text{in}} < 0, \tag{86}$$

$$\mathcal{Q}_{22}^{\text{out}} = R\frac{\langle \hat{n}_1^2 \rangle - \langle \hat{n}_1 \rangle^2}{\langle \hat{n}_1 \rangle} + T - 1 = R\frac{\langle \hat{n}_1^2 \rangle - \langle \hat{n}_1 \rangle^2}{\langle \hat{n}_1 \rangle} - R = R\mathcal{Q}_{11}^{\text{in}} < 0, \tag{87}$$

where we have used the fact that $R + T = 1$ and that the input Mandel Q parameter is as follows:

$$\mathcal{Q}_{11}^{\text{in}} = \frac{\langle \hat{n}_1^2 \rangle - \langle \hat{n}_1 \rangle^2}{\langle \hat{n}_1 \rangle} - 1. \tag{88}$$

Clearly, the sub-Poissonian statistics were redistributed accordingly to transmissivity. Now, it is straightforward to obtain the following particularly important relation:

$$\mathcal{Q}_{12}^{\text{out}} + \mathcal{Q}_{21}^{\text{out}} = \mathcal{Q}_{11}^{\text{in}}. \tag{89}$$

This shows that, starting from the product input state (80), the two-mode entanglement after beam splitting is exclusively inherited from the sub-Poissonian statistics of the input state. Therefore, beam splitting redistributes the internal non-classical photon number correlation of the state to the photon number entanglement of the output modes. Note that due to this equality, $\mathcal{Q}_{12}^{\text{out}} + \mathcal{Q}_{21}^{\text{out}}$ is lower bounded by -1 and minimized by the input states being Fock states $\hat{\rho}_\varphi = |n\rangle\langle n|$.

8. Concluding remarks

In summary, we have proposed an extension of the reduced state of the field formalism for mesoscopic bosonic fields. Our extension allows for tracking the evolution of particle number entanglement for systems undergoing non-unitary Markovian evolution, which is not possible in the original reduced state of the field approach. The extended approach allows for studying entanglement of both Gaussian and non-Gaussian states. This was achieved by reducing the problem of entanglement of multi-mode bosonic state into the entanglement of the two-particle state on a finite-dimensional Hilbert space. Based on the proposed approach, we showed that particle number entanglement of multi-mode bosonic field is independent of the efficiency of the detectors if it is the same across all detectors. Moreover, we showed that the entanglement of the states of the beam-splitted single photon and 2×2 bright squeezed vacuum are robust against interaction with a low-temperature thermal environment. Furthermore, we considered the generalization of the Mandel Q parameter constructed within the proposed approach, which describes non-classical correlations both in a single mode and shared among different modes. Using this parameter, we showed that the entanglement of two-mode entangled states obtained by the beam splitting of one occupied mode is solely inherited from the sub-Poissonian statistics of the input state.

The proposed reduced state of the field description can provide a versatile and intuitive tool for the analysis of the impact of decoherence on non-classical phenomena in multiple optical experimental setups and consequently their designing. This is because our approach inherits multiple tools from standard quantum mechanics of finite-dimensional systems, with only a slight change in interpretation. As analysis of a given setup requires only specifying mesoscopic properties of the sources instead of the whole initial state, it could be done without even invoking the Fock space. Furthermore, one can easily incorporate passive optical elements and inefficiencies in the description of the evolution. In addition, ancillary modes and entanglement can also be added to the system through the use of beamsplitters.

One of the important limitations of proposed formalism is the class of accessible evolution equations. This class is restricted to master equations with terms that are at most linear in the creation and annihilation operators. Often, it is possible to transform the considered problem into the problem described by such evolution through employing, e.g. Bogoliubov transformations of modes and through simplifying interactions using the mean field. However, if one wants to transform back to the original modes, one has to consider the evolution of additional structures. This is because the information contained in ρ_4 is insufficient. Alternatively to Bogoliubov transformations, one can directly calculate the evolution of ρ_4 for quadratic Hamiltonians by including the additional structures mentioned above (see appendix C). However, for higher-order interactions, one needs to track higher-order correlations in order to propose a sensible approximate set of closed evolution equations. Still, whenever one cannot use the convenient evolution equations for the reduced state described in this work, one can use the extended reduced state in the analysis of non-classical features of the state. Another limitation of the formalism is that it is restricted to two-party entanglement and that entanglement of the reduced state is only a sufficient criterion for entanglement. Nevertheless, one can build analogously reduced three- and more-particle-like states and upon it consider more involved types of entanglement.

Let us also note that since the extended reduced state of the field preserves a state-like interpretation of reduced states and maintains a Hilbert space structure for them, one can exploit scalar product of these Hilbert spaces for geometric-like considerations of bosonic states as, e.g. in [55]. This allows for considerations of proximity of states in terms of reduced states and therefore for their classification in terms of mesoscopic properties.

As we found that for both single-photon entangled state and bright squeezed vacuum the entanglement is robust against thermal damping in low temperatures, an interesting open question arises. Is this property universal to photon number entanglement?

The proposed extension of the reduced state of the field approach could also be used to examine different quantum optical phenomena. Let us recall that the original reduced state of the field contained information about the expectation values of Stokes operators, providing a generalization to the description of polarization in terms of Jones vectors. Our extension, when restricted to two modes, additionally keeps information about second-order polarization tensors [32, 56]. As these tensors are associated with non-classical phenomena of hidden polarization, our approach could give additional insight into this phenomenon.

Data availability statement

No new data were created or analysed in this study.

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Appendix A. Lack of entanglement detection of beam-splitted single photon by PPT criterion applied to covariance matrix

Let us show that the PPT criterion applied to the covariance matrix does not allow for the detection of entanglement of the state of single photon beam splitted into two modes a_1 and a_2:

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(|1;0\rangle + |0;1\rangle) = \frac{1}{\sqrt{2}}\left(\hat{a}_1^\dagger + \hat{a}_2^\dagger\right)|\Omega\rangle. \tag{A.1}$$

Let us recall that covariance matrix is given by:

$$V_{i,j} = \frac{1}{2}\left\langle\left\{\hat{\Xi}_i, \hat{\Xi}_j\right\}\right\rangle - \langle\hat{\Xi}_i\rangle\langle\hat{\Xi}_j\rangle, \tag{A.2}$$

where $\vec{\Xi} = (\hat{x}_1, \hat{p}_1, \ldots, \hat{x}_n, \hat{p}_n)$ and operators $\hat{x}_j, \hat{p}_j$ are dimensionless position and momentum operators in jth mode:

$$\hat{x}_j = \frac{1}{\sqrt{2}}\left(\hat{a}_j + \hat{a}_j^\dagger\right), \quad \hat{p}_j = \frac{i}{\sqrt{2}}\left(\hat{a}_j^\dagger - \hat{a}_j\right). \tag{A.3}$$

By noting that for state (A.1) we have $\langle\hat{a}_j^\dagger\rangle = \langle\hat{a}_j\rangle = \langle\hat{a}_j^\dagger\hat{a}_i^\dagger\rangle = \langle\hat{a}_j\hat{a}_i\rangle = 0$ and $\langle\hat{a}_j^\dagger\hat{a}_i\rangle = 1/2$, one can write down the covariance matrix for this state as:

$$V = \frac{1}{2}\begin{pmatrix} \langle 2\hat{a}_1^\dagger\hat{a}_1\rangle + 1 & 0 & \langle\hat{a}_1^\dagger\hat{a}_2 + \hat{a}_2^\dagger\hat{a}_1\rangle & 0 \\ 0 & \langle 2\hat{a}_1^\dagger\hat{a}_1\rangle + 1 & 0 & \langle\hat{a}_1^\dagger\hat{a}_2 + \hat{a}_2^\dagger\hat{a}_1\rangle \\ \langle\hat{a}_1^\dagger\hat{a}_2 + \hat{a}_2^\dagger\hat{a}_1\rangle & 0 & \langle 2\hat{a}_2^\dagger\hat{a}_2\rangle + 1 & 0 \\ 0 & \langle\hat{a}_1^\dagger\hat{a}_2 + \hat{a}_2^\dagger\hat{a}_1\rangle & 0 & \langle 2\hat{a}_2^\dagger\hat{a}_2\rangle + 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2 & 0 & 1 & 0 \\ 0 & 2 & 0 & 1 \\ 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 2 \end{pmatrix}. \tag{A.4}$$

The PPT criterion for entanglement in terms of the covariance matrix is given as follows:

$$Q\cdot V\cdot Q - \frac{i}{2}J < 0, \tag{A.5}$$

where $Q = \mathrm{diag}(1, q_1, \ldots, 1, q_n)$ with $q_j = -1$ for modes corresponding to transposed subsystem and $q_j = 1$ otherwise, and:

$$J = \bigoplus_{k=1}^{n} J_2, \quad J_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{A.6}$$

This criterion is necessary and sufficient condition for detecting two mode entanglement of Gaussian states and sufficient condition for non-Gaussian states (which is a the case for (A.1)). The eigenvalues of the matrix on the r.h.s. of inequality (A.5) for the state (A.1) are positive and equal to $(2\pm\sqrt{2})/2$. Therefore, one does not find entanglement with PPT criterion applied to the covariance matrix of the state (A.1).

Appendix B. Extending reduce states by separable subsystems

Often when one wants to consider multiple modes with the states of different modes prepared by different sources. In such a case, the total state is a product state of subsystems. Let us consider the case of two subsystems A and B with total state $\rho_{\mathrm{tot}} = \hat{\rho}_A \otimes \hat{\rho}_B$. It is often easier to construct the reduced state of the total state using the simpler reduced states of $\hat{\rho}_A$ and $\hat{\rho}_B$. This is possible as for such states we have $\langle\hat{A}\hat{B}\rangle = \langle\hat{A}\rangle\langle\hat{B}\rangle$, where $\hat{A}, \hat{B}$ are some observables on modes corresponding to subsystems A and B. The reduced state of the whole system can then be obtained as follows:

$$\begin{aligned}
|\alpha_t\rangle &= |\alpha_A\rangle + |\alpha_B\rangle,\\
\hat{\rho}_t &= \hat{\rho}_A + \hat{\rho}_B + |\alpha_A\rangle\langle\alpha_B| + |\alpha_B\rangle\langle\alpha_A|,\\
\hat{r}_t &= \hat{r}_A + \hat{r}_B + |\alpha_A\rangle\langle\alpha_B^*| + |\alpha_B\rangle\langle\alpha_A^*|,\\
\hat{\beta}_t &= \hat{\beta}_A + (|\alpha_A^*\rangle\hat{r}_B)^{T_1} + (|\alpha_B\rangle\hat{\rho}_A)^{\tau_L} + A \leftrightarrow B,\\
\hat{\rho}_{4t} &= \hat{\rho}_{4A} + \hat{\beta}_A\langle\alpha_B| + (\hat{\beta}_A\langle\alpha_B| - |\alpha_A\rangle\langle\alpha_B| \otimes \mathbf{1} + |\alpha_B\rangle\hat{\beta}_A^\dagger)^{\tau_R}\\
&\quad + (|\alpha_B\rangle(\hat{\beta}_A^\dagger)^{\tau_R} - |\alpha_B\rangle\langle\alpha_A| \otimes \mathbf{1})^{\tau_L} + A \leftrightarrow B,
\end{aligned} \tag{B.1}$$

where subscript t stands for the total state and indices A and B for the corresponding parties. Note that swap operations τ_L, τ_R can be performed using $N^2 \times N^2$-dimensionl matrix $\hat{\tau}$, where N is total number of modes:

$$\tau_{i,j} = \begin{cases} 1 & \exists m, n \in \{1 \ldots, d\} : \ i = m + d(-1+n) \text{ and } j = d(-1+m) + n \\ 0 & \text{otherwise} \end{cases}. \tag{B.2}$$

Then, for some operator $\hat{O}$, one gets:

$$O^{\tau_L} = \hat{\tau}\hat{O}, \tag{B.3}$$

$$O^{\tau_R} = \hat{O}\hat{\tau}. \tag{B.4}$$

Appendix C. Full second-order evolution

In a manner similar to the presented extended RSF approach, one could consider the full second-order evolution of the system. In such a scenario, one could consider reduction of the second-order observables to three reduced operators on single particle space:

$$\begin{aligned}
\hat{O} &:= \sum_{k,k'} o_{k,k'}\hat{a}_k^\dagger\hat{a}_{k'} + \frac{1}{2}\sum_{k,k'}\left(q_{k,k'}\hat{a}_k\hat{a}_{k'} + q_{k,k'}^*\hat{a}_k^\dagger\hat{a}_{k'}^\dagger\right)\\
&\to \left(\hat{o} = \sum_{k,k'} o_{k,k'}|k\rangle\langle k'|, \hat{q} := \frac{1}{2}\sum_{k,k'}(q_{k,k'})\,|k\rangle\langle k'|, \hat{q}^* := \frac{1}{2}\sum_{k,k'}\left(q_{k,k'}^*\right)|k\rangle\langle k'|\right).
\end{aligned} \tag{C.1}$$

Note that reducing also first-order observables:

$$\hat{O}' = \sum_k\left(p_k\hat{a}_k + p_k^*\hat{a}_k^\dagger\right) \to \left(\langle p| := \sum_k p_k\langle k|, \langle p^*| := \sum_k p_k^*\langle k|\right), \tag{C.2}$$

the expectation value of the combination of such observables is given by:

$$\langle\hat{O}\rangle + \langle\hat{O}'\rangle = \mathrm{Tr}\,\hat{O}\hat{\rho}_F = \mathrm{tr}\,(\hat{o}, \hat{q}, \hat{q}^*) \cdot (\hat{\rho}, \hat{r}, \hat{r}^*)^T + (\langle p|, \langle p^*|) \cdot (|\alpha\rangle, |\alpha^*\rangle)^T. \tag{C.3}$$

We can now allow any Hamiltonian that can be reduced by the procedure (C.1). We denote the reduced Hamiltonian by the following triple $(\hat{h}, \hat{h}_s, \hat{h}_s^*)$. The operator $\hat{h}$ governs the free evolution and exchange of photons between modes, whereas the operators $\hat{h}_s, \hat{h}_s^*$ correspond to single-mode and two-mode squeezing. Introducing such an interaction Hamiltonian can correspond, e.g. to using a parametric approximation to some modes in the system. These modes are treated as classical coherent pumping fields which are subject to, e.g. a parametric down-conversion process in which annihilation of a single photon from the pumping field is accompanied by creation of two photons in modes which we treat in a full quantum manner. This addition to the formalism is similar to the addition of coherent pumping in (6). However, such an extended evolution requires an extension of the reduced states. If one is only interested in the evolution of the original reduced state $\hat{\rho}$ the addition of $\hat{r}$ is sufficient. Then, one can analogously obtain equations of motion for RSF, which are the following:

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho} = -\frac{i}{\hbar}\left[\hat{h}, \hat{\rho}\right] - \frac{2i}{\hbar}\left(\hat{h}_s^*\hat{r}^* - \hat{r}\hat{h}_s\right) + (|\xi\rangle\langle\alpha| + |\alpha\rangle\langle\xi|) + \frac{1}{2}\{\hat{\gamma}_\uparrow - \hat{\gamma}_\downarrow^T, \hat{\rho}\} + \hat{\gamma}_\uparrow, \tag{C.4}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{r} = -\frac{i}{\hbar}\hat{h}\hat{r} - \frac{2i}{\hbar}\hat{h}_s^*\hat{\rho}^T - \frac{i}{\hbar}\hat{h}_s^* + |\xi\rangle\langle\alpha^*| + \frac{1}{2}\left(\hat{\gamma}_\uparrow - \hat{\gamma}_\downarrow^T\right)\hat{r} + T., \tag{C.5}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}|\alpha\rangle = -\frac{i}{\hbar}\hat{h}|\alpha\rangle - \frac{2i}{\hbar}\hat{h}_s^*|\alpha\rangle + |\xi\rangle + \frac{1}{2}\left(\hat{\gamma}_\uparrow - \hat{\gamma}_\downarrow^T\right)|\alpha\rangle, \tag{C.6}$$

where 'T.' stands for the transposed expression. To consider the evolution of $\hat{\rho}_4$, one needs to extend the reduction by the additional reduced states:

$$\hat{m} := \sum_{k_1,k_2,k_3,k_4} \mathrm{tr}\,\hat{\rho}_F \hat{a}_{k_1}^\dagger \hat{a}_{k_2}\hat{a}_{k_3}\hat{a}_{k_4}|k_2,k_4\rangle\langle k_1,k_3|, \tag{C.7}$$

$$\hat{q} := \sum_{k_1,k_2,k_3,k_4} \mathrm{tr}\,\hat{\rho}_F \hat{a}_{k_1}\hat{a}_{k_2}\hat{a}_{k_3}\hat{a}_{k_4}|k_2,k_4\rangle\langle k_1,k_3|, \tag{C.8}$$

$$\hat{\zeta} := \sum_{k_1,k_2,k_3,k_4} \mathrm{tr}\,\hat{\rho}_F \hat{a}_{k_1}\hat{a}_{k_2}\hat{a}_{k_3}|k_2,k_3\rangle\langle k_1|. \tag{C.9}$$

Then, the set of evolution equations is extended by:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_4 = &-\frac{i}{\hbar}\left[\hat{h}\otimes\mathbf{1}+\mathbf{1}\otimes\hat{h},\hat{\rho}_4\right] - \frac{2i}{\hbar}\left(\mathbf{1}\otimes\hat{h}_s^\dagger\hat{m}^\dagger + \left(\mathbf{1}\otimes\hat{h}_s^\dagger\hat{m}^\dagger\right)^{\tau_L} - \hat{m}\mathbf{1}\otimes\hat{h}_s - \left(\hat{m}\mathbf{1}\otimes\hat{h}_s\right)^{\tau_R}\right)\\ &-\frac{2i}{\hbar}\left(\left(\hat{h}_s^\dagger\hat{r}^\dagger\otimes\mathbf{1}\right)^{\tau_L} + \left[\left(\hat{r}^\dagger\otimes\hat{h}_s^\dagger\right)^{\tau_L}\right]^{T_2} - \left(\hat{r}\hat{h}_s\otimes\mathbf{1}\right)^{\tau_L} - \left[\left(\hat{h}_s\otimes\hat{r}\right)^{\tau_L}\right]^{T_2}\right)\\ &+\left(|\xi\rangle\hat{\beta}^\dagger + \left(|\xi\rangle\hat{\beta}^\dagger\right)^{\tau_L} + \left(|\xi\rangle\langle\alpha|\otimes\mathbf{1}\right)^{\tau_L} + \hat{\beta}\langle\xi| + \left(\hat{\beta}\langle\xi|\right)^{\tau_R} + \left(\mathbf{1}\otimes|\alpha\rangle\langle\xi|\right)^{\tau_R}\right)\\ &+\frac{1}{2}\left\{\left(\mathbf{1}\otimes\hat{\gamma}_\uparrow+\hat{\gamma}_\uparrow\otimes\mathbf{1}\right) - \left(\mathbf{1}\otimes\hat{\gamma}_\downarrow^T+\hat{\gamma}_\downarrow^T\otimes\mathbf{1}\right),\hat{\rho}\right\}\\ &+\left(\hat{\rho}\otimes\gamma_\downarrow^T\right)^{\tau_L} + \left(\gamma_\uparrow\otimes\hat{\rho}\right)^{\tau_L} + \gamma_\uparrow\otimes\hat{\rho} + \hat{\rho}\otimes\gamma_\uparrow + \left(\gamma_\uparrow\otimes\mathbf{1}\right)^{\tau_L},\end{aligned} \tag{C.10}$$

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\hat{m} = &-\frac{i}{\hbar}\left[\hat{h}\otimes\mathbf{1},\hat{m}\right] - \frac{i}{\hbar}\left(\mathbf{1}\otimes\hat{h}\hat{m} + \hat{m}\mathbf{1}\otimes\hat{h}^T\right) - \frac{2i}{\hbar}\left(\hat{\rho}_4\mathbf{1}\otimes\hat{h}_s^\dagger + \left\{\mathbf{1}\otimes\hat{h}_s^\dagger,\hat{\rho}_4\right\}^{T_2} - \hat{q}\hat{h}_s\otimes\mathbf{1}\right)\\ &-\frac{2i}{\hbar}\left(\hat{\rho}\otimes h_s^\dagger - \left[\left(\hat{\rho}\otimes h_s^\dagger\right)^{\tau_L}\right]^{T_2}\right) + \left(\hat{\beta}\langle\xi^*| + \left(\hat{\beta}\langle\xi^*|\right)^{T_2} + \left[\left(\hat{\beta}\langle\xi^*|\right)^{T_2}\right]^{\tau_L} + \left(\hat{\zeta}\langle\xi|\right)^{\tau_R}\right)\\ &+\frac{1}{2}\left\{\left(\hat{\gamma}_\uparrow\otimes\mathbf{1}\right) - \left(\hat{\gamma}_\downarrow^T\otimes\mathbf{1}\right),\hat{m}\right\} + \frac{1}{2}\left(\mathbf{1}\otimes\hat{\gamma}_\uparrow\hat{m} + \hat{m}\mathbf{1}\otimes\hat{\gamma}_\uparrow^T - \mathbf{1}\otimes\hat{\gamma}_\downarrow^T\hat{m} - \hat{m}\mathbf{1}\otimes\hat{\gamma}_\downarrow\right)\\ &+\hat{\gamma}_\uparrow\otimes\hat{r} + \left(\hat{\gamma}_\uparrow\otimes\hat{r}\right)^{\tau_L} + \left[\left(\hat{\gamma}_\uparrow\otimes\hat{r}\right)^{\tau_L}\right]^{T_2},\end{aligned} \tag{C.11}$$

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\hat{q} = &-\frac{i}{\hbar}\left(\hat{h}\otimes\mathbf{1}\hat{q} + \hat{q}\hat{h}^T\otimes\mathbf{1} + \mathbf{1}\otimes\hat{h}\hat{q} + \hat{q}\mathbf{1}\otimes\hat{h}^T\right)\\ &-\frac{2i}{\hbar}\left(\left(\hat{h}_s^\dagger\otimes\mathbf{1}\hat{m}^T\right)^{\tau_L} + \left(\hat{m}\hat{h}_s^\dagger\otimes\mathbf{1}\right)^{\tau_R} + \hat{h}_s^\dagger\otimes\mathbf{1}\hat{m} + \hat{m}^T\hat{h}_s^\dagger\otimes\mathbf{1}\right)\\ &-\frac{2i}{\hbar}\left(\hat{r}\otimes\hat{h}_s^\dagger + \left(\hat{r}\otimes\hat{h}_s^\dagger\right)^{\tau_L} + \left[\left(\hat{r}\otimes\hat{h}_s^\dagger\right)^{\tau_L}\right]^{T_2}\right) - \frac{2i}{\hbar}\left(\hat{h}_s^\dagger\otimes\hat{r} + \left(\hat{h}_s^\dagger\otimes\hat{r}\right)^{\tau_L} + \left[\left(\hat{h}_s^\dagger\otimes\hat{r}\right)^{\tau_L}\right]^{T_2}\right)\\ &+\left(\hat{\zeta}\langle\xi^*| + \left(\hat{\zeta}\langle\xi^*|\right)^{T_2} + \left(\hat{\zeta}\langle\xi^*|\right)^{\tau_R} + \left[\left(\hat{\zeta}\langle\xi^*|\right)^{\tau_R}\right]^{T_1}\right)\\ &+\frac{1}{2}\left(\hat{\gamma}_\uparrow\otimes\mathbf{1} + \mathbf{1}\otimes\hat{\gamma}_\uparrow - \hat{\gamma}_\downarrow^T\otimes\mathbf{1} - \mathbf{1}\otimes\hat{\gamma}_\downarrow^T\right)\hat{q} + \frac{1}{2}\hat{q}\left(\hat{\gamma}_\uparrow^T\otimes\mathbf{1} + \mathbf{1}\otimes\hat{\gamma}_\uparrow^T - \hat{\gamma}_\downarrow\otimes\mathbf{1} - \mathbf{1}\otimes\hat{\gamma}_\downarrow\right),\end{aligned} \tag{C.12}$$

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\hat{\beta} = &-\frac{i}{\hbar}\left[\hat{h}\otimes\mathbf{1},\hat{\beta}\right] - \frac{i}{\hbar}\mathbf{1}\otimes\hat{h}\hat{\beta}\\ &-\frac{2i}{\hbar}\left(\left(\hat{\beta}^\dagger\mathbf{1}\otimes\hat{h}_s^\dagger\right)^{T_2} + \left[\left(\hat{\beta}^\dagger\mathbf{1}\otimes\hat{h}_s^\dagger\right)^{T_2}\right]^{\tau_L} + \left[\left(\hat{h}_s^\dagger\otimes\langle\alpha|\right)^{\tau_R}\right]^{T_2} - \hat{\zeta}\hat{h}_s\otimes\mathbf{1}\right)\\ &+\left(\hat{\rho}\otimes|\xi\rangle + \left(\hat{\rho}\otimes|\xi\rangle\right)^{\tau_L} + \left[\left(\hat{r}\otimes\langle\xi|\right)^{\tau_R}\right]^{T_2}\right)\\ &+\frac{1}{2}\left(\left\{\hat{\gamma}_\uparrow\otimes\mathbf{1} - \hat{\gamma}_\downarrow^T\otimes\mathbf{1},\hat{\beta}\right\} + \left(\mathbf{1}\otimes\hat{\gamma}_\uparrow - \mathbf{1}\otimes\hat{\gamma}_\downarrow^T\right)\hat{\beta}\right) + \hat{\gamma}_\uparrow\otimes|\alpha\rangle + \left(\hat{\gamma}_\uparrow\otimes|\alpha\rangle\right)^{\tau_L},\end{aligned} \tag{C.13}$$

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\hat{\zeta} = &-\frac{i}{\hbar}\left[\hat{h}\otimes\mathbf{1}\hat{\zeta}+\hat{\zeta}\hat{h}^{T}\otimes\mathbf{1}+\mathbf{1}\otimes\hat{h}\hat{\zeta}\right]-\frac{2i}{\hbar}\left(\hat{\beta}\hat{h}_s^{\dagger}\otimes\mathbf{1}+\hat{h}_s^{\dagger}\otimes\mathbf{1}\hat{\beta}^{T_1}+\left(\hat{h}_s^{\dagger}\otimes\mathbf{1}\hat{\beta}^{T_1}\right)^{\tau_L}\right)\\ &-\frac{2i}{\hbar}\left(\hat{h}_s^{\dagger}\otimes|\alpha\rangle+\left(\hat{h}_s^{\dagger}\otimes|\alpha\rangle\right)^{\tau_L}+\left[\left(\hat{h}_s^{\dagger}\otimes|\alpha\rangle\right)^{\tau_L}\right]^{T_1}\right)\\ &+\left(\hat{r}\otimes|\xi\rangle+(\hat{r}\otimes|\xi\rangle)^{\tau_L}+[(\hat{r}\otimes|\xi\rangle)^{\tau_L}]^{T_1}\right)\\ &+\frac{1}{2}\left(\left(\hat{\gamma}_{\uparrow}\otimes\mathbf{1}-\hat{\gamma}_{\downarrow}^{T}\otimes\mathbf{1}\right)\hat{\zeta}+\hat{\zeta}\left(\hat{\gamma}_{\uparrow}^{T}\otimes\mathbf{1}-\hat{\gamma}_{\downarrow}\otimes\mathbf{1}\right)+\left(\mathbf{1}\otimes\hat{\gamma}_{\uparrow}-\mathbf{1}\otimes\hat{\gamma}_{\downarrow}^{T}\right)\hat{\zeta}\right).\end{aligned}\tag{C.14}$$

Note that such an extended RSF allows for calculation of any additive observable up to fourth the order in creation and annihilation operators.

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