Atomic boson sampling in a Bose-Einstein-condensed gas

V. V. Kocharovsky,[1] Vl. V. Kocharovsky,[2] and S. V. Tarasov[2]
[1]*Department of Physics and Astronomy, Texas A&M University, College Station, Texas 77843, USA*
[2]*Institute of Applied Physics, Russian Academy of Sciences, Nizhny Novgorod 603950, Russia*

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We consider quantum statistical physics of many-body equilibrium fluctuations in an interacting Bose-Einstein-condensed (BEC) gas. We find a universal analytic formula for a characteristic function (Fourier transform) of a joint probability distribution for the particle occupation numbers in a BEC gas and discuss ♯P-hardness of computing this distribution. The latter is done by means of the Hafnian master theorem generalizing the classical permanent master theorem of MacMahon. We suggest an atomic boson sampling in the many-body interacting systems as an alternative to a widely studied Gaussian boson sampling of photons. We outline a multiqubit BEC trap, formed by a set of the single-qubit potential wells, as a convenient model for studying atomic boson sampling.

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I. INTRODUCTION: MANY-BODY BEC FLUCTUATIONS AND GAUSSIAN BOSON SAMPLING

The subject of the paper is the quantum statistical physics of the many-body equilibrium fluctuations in a gas with a Bose-Einstein condensate (BEC). We present the explicit analytic solution for the statistics of this stationary stochastic process and associated atomic boson sampling. In doing this analysis, we need to touch, albeit only briefly, upon a prototype model and experimental aspects of atomic boson sampling in a BEC gas as well as upon mathematics behind a computational complexity of the above process. Those aspects of this nontrivial physical problem are closely related to the fundamental physics of the many-body process under consideration. Their detailed analysis is certainly needed, but it is beyond the scope of the present paper.

Boson sampling of the single-photon Fock states in a linear interferometer had been suggested in Refs. [1,2] for demonstrating quantum advantage of many-body quantum simulators over classical computers [3–7]. Yet an absence of suitable on-demand sources of single photons put forward the boson sampling of Gaussian, squeezed states of photons as the most plausible platform [2,8–32]. We consider physics of an alternative system which is based on the BEC of trapped interacting atoms. The starting point of our analysis is a fact of two-mode squeezing of particle excitations in a BEC trap established in Ref. [33] and strongly pronounced in the fluctuations of a total BEC occupation calculated in Ref. [34].

Physics of N atoms in a BEC trap looks substantially different from the physics of massless photons in the interaction-free, nonequilibrium (nonthermal), linear interferometer due to the presence of the condensate, thermal equilibrium, particle mass, and interaction as well as the absence of external sources of bosons. Yet we show that these peculiarities do not prevent us from solving this problem analytically and, in fact, turn the BEC trap into a deep platform for testing quantum many-body physics, in particular, boson sampling. In the present paper, we elaborate on the underlying many-body BEC physics and do not aim to simulate the Gaussian boson sampling in an optical interferometer.

Consider joint fluctuations in the occupations of the excited particle states. We find a truly simple, universal formula for their characteristic function (Fourier transform of their joint probability distribution) in terms of a normally ordered correlation function G of trapped particles. By means of the Hafnian master theorem (28), it yields the cumulants (hence, moments) and probabilities of the joint distribution via a matrix Hafnian (a certain extension of the matrix permanent [35–37]). The Hafnians and permanents are ♯P-hard for computing [38,39] and can be viewed as a universal tool for analyzing the ♯P-hard problems [3,40]. This fact implies ♯P-hardness of computing many-body equilibrium fluctuations in the occupations of excited particle states in a BEC trap and opens a path for the exploration of an entire spectrum of the theoretical or experimental BEC problems inspired by boson sampling in an optical interferometer.

A reduction to computing a permanent is known also for the transition amplitude of a quantum circuit in a universal quantum computer [41]. This fact puts the ♯P-hardnesses of (i) the quantum statistics in a BEC trap and (ii) the universal quantum computer on the same footing.

For simplicity's sake, we consider an equilibrium BEC in a weakly interacting gas at temperatures well below the critical region within the Bogoliubov-Popov approximation [42,43] and show that computing particle excitation fluctuations is a ♯P-hard problem (even within the grand canonical ensemble adopted in this paper).

The grand canonical ensemble does not fully account for the canonical-ensemble constraint of an exact conservation of the total number of particles N in the BEC trap, $N = \text{const}$. The latter is the ultimate reason for the very onset of the BEC phase transition [44]. A canonical-ensemble analysis of the critical fluctuations near the critical temperature of the BEC

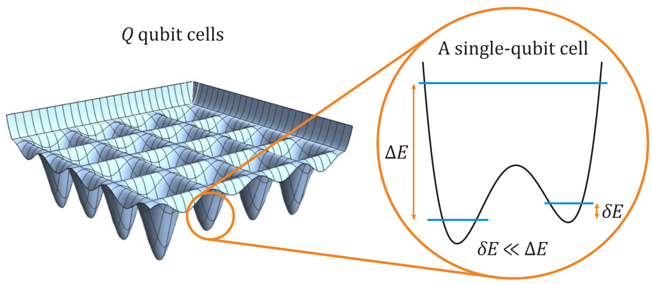

FIG. 1. The multiqubit BEC trap: A sketch of the geometry of its trapping potential in the case of a two-dimensional lattice built of the Q single-qubit cells. Each single-qubit cell is formed by a double-well potential featuring two close lower energy levels separated from the higher energy levels by the energy gap ΔE much wider than the lower-energy splitting δE. Slightly uneven depths of different single-qubit cells are chosen on purpose to show the presence of an inhomogeneous underlying (background) potential, designed for controlling cell occupations, the condensate profile, and Bogoliubov couplings. For clarity's sake, the high potential walls at the outer borders of the multiqubit trap are not shown.

phase transition is much more involved. It can be fulfilled on the basis of the Holstein-Primakoff, or Girardeaux-Arnowitt, representation by means of the nonpolynomial diagram technique and recurrence equations for partial contractions of the atomic field operators described in Refs. [45–47]. It also leads to the matrix permanent or Hafnian.

Experimental studies of cold dilute gases [48–62] allowed one to directly measure fluctuations in a total noncondensate occupation. Further splitting the noncondensate into parts and measuring fluctuations in occupations of the coarse-grained groups of excited states will come soon. Understanding such fluctuations means reaching a much deeper level of quantum statistics than a level of the mean condensate, quasiparticle characteristics, and condensate fluctuations studied previously [50,51,63–68]. Particle-number fluctuations are important for matter-wave interferometers [69] (like Ramsey [70,71] or Mach-Zehnder [72] on-chip ones) and were studied for squeezed states [70] and trap cells [73,74].

II. A POTENTIAL TRAP DESIGN FEATURING ATOMIC BOSON SAMPLING: THE BEC TRAP MADE UP OF QUBIT POTENTIAL WELLS

To exemplify a many-body system under general physical analysis, let us use an example shown in Fig. 1. Such specially designed traps could be employed to test atomic boson sampling in a controllable, full, and clear way. The challenge is twofold. First, a trap with a finite number M of lower split-off excited states or groups of states, coupled to each other via Bogoliubov coupling, is desirable. If all higher excited states are separated from such a lower miniband by an energy gap wider than the temperature T and have vanishing Bogoliubov couplings, they have exponentially small occupations and can be skipped or accounted for as a kind of perturbation. Second, there should be a way to sample and simultaneously measure occupations of some lower miniband states or some groups of them, say, via a multidetector imaging.

Consider a design of the BEC trap with a split-off lower energy miniband inspired by an analogy with a multiqubit system. Let us start with several, Q, tight qubit cells, each with two close lower energy levels, adjust the intercell potential barriers to be relatively narrow but not very high, and arrange the cells into a two- or three-dimensional lattice. Then, place the lattice on top of a slightly varying in space background potential with high walls at the trap borders. Quantum tunneling of atoms under the intercell barriers should be significant to ensure a reasonable interaction between atoms from different individual qubit wells needed for a formation of a common nonuniform condensate and significant Bogoliubov couplings within a large subset of excited states. Otherwise, the atomic boson sampling would not show its full computational complexity.

If the intercell potential walls are infinitely high and cells are the same, then two wave eigenfunctions corresponding to the first, e_1, and second, e_2, energy levels in each single-qubit cell constitute a natural basis for constructing the excited states of the trap. The 2^Q combinations of those single-qubit states are the eigenfunctions of the entire multiqubit well and form a lower miniband of energy levels, $\{\varepsilon_q\}$. In the degenerate case of the identical single-qubit cells, there are $Q+1$ different levels in this miniband, $\varepsilon_q = (Q-q)e_1 + qe_2$; $q = 0, 1, ..., Q$. A degeneracy, g_q, of each level ε_q is the number of ways to assign the second energy level e_2 to the q single-qubit cells and the first energy level e_1 to the rest of the $Q-q$ single-qubit cells, that is, the binomial coefficient, $g_q = \binom{Q}{q}$. The sum of those degeneracies equals the total number of wave eigenfunctions in the miniband, $\sum_{q=0}^{Q}\binom{Q}{q} = 2^Q$.

It is instructive to see how these eigenfunctions of the multiqubit trap with infinitely high walls emerge adiabatically from single-particle wave functions of the original structureless (say, box) trap with increasing intercell potentials. Analysis of a one-dimensional (1D) model with a flat potential and almost equally spaced delta-function potential barriers suggests that these eigenfunctions in the system of independent qubit cells asymptotically correspond to the appropriate superpositions of the $2Q$ lower-energy eigenfunctions of the entire trap with finite potential barriers. Based on this observation, one can choose the $2Q$ lower-energy eigenfunctions of an actual trap as a system of two ($s=1$ and $s=2$) bands of the generating eigenfunctions $\{\varphi_{s,p}|p=1,...,Q\}$ to work with. By analogy, it is even possible to think about a new system of Q distributed qubits assigning a pair of eigenfunctions $\varphi_{1,p}$ and $\varphi_{2,p'}$ (e.g., with equal indices $p'=p$) to be the lower and upper energy states of a new qubit. In such a multiqubit model of an actual trap with arbitrary finite (not necessarily infinite) intercell potential walls, there are 2^Q multiqubit combinations of the above eigenfunctions of the miniband of the $2Q$ lowest energy levels. The corresponding qubits are not identical anymore, even if the cell dimensions are the same.

Varying the dimensions and background potentials of the single-qubit cells would allow one to control and vary the trap eigenfunctions $\varphi_{s,p}$ and energy levels in a wide range. In particular, the background potentials individually control the amplitudes of eigenfunctions in different cells, that is, the relative occupations of different single-qubit cells. Tuning the intracell potential barriers provides an efficient tool for controlling the intraqubit properties such as the qubit energy splittings δE_j, $j = 1, ..., Q$.

In this paper, we consider an arbitrary number, $M + 1$, of the single-particle energy levels of the trap constituting a miniband. For example, one can adjust parameters to have a lower miniband of $M + 1 = 2Q$ levels separated from all higher energy levels by an energy gap ΔE wider than the temperature T. In a typical design, the size of the qubit well is of the order of the de Broglie wavelength, about 1 μm. The size of the entire multiqubit BEC trap, say, in the 2D case is about $\sqrt{Q}$ μ*m*.

Another design could be based on a bunch of Q quasi-1D BEC traps each supporting a preselected (say, via a properly designed Bragg reflection) longitudinal atomic mode and coupled to neighbors via a quantum tunneling through potential barriers constituting walls between 1D traps. A cross-section profile of each 1D trap could support two, almost degenerate, transverse atomic modes with close lower energy levels constituting a qubit for each longitudinal mode. All higher-order transverse atomic modes could have much higher energy levels separated from the two qubit levels by a gap $\Delta E \gg T$.

An individual qubit well has a twofold-degenerate ground level split by a certain perturbation. In particular, a double-well trap becomes the qubit well if its parameters are adjusted appropriately. BEC in the double-well traps and optical lattices as well as their Bogoliubov excitations are well studied [63,69,70,75–81].

Lowering the temperature below the critical value T_c and controlling the inhomogeneous background potential and barriers separating qubit wells allow one to create an entire hierarchy of BEC regimes [78]: From the regime of anomalously large critical fluctuations in the critical region (neat T_c) or strongly correlated regime to the regime of a quasicondensate or fragmented condensates of the individual qubit wells to the regime of a well established, macroscopically occupied common condensate inhomogeneously spread over the entire trap at $T \ll T_c$. We consider the latter case assuming $N \gg Q$.

Note that at $T \ll T_c$ the excited states above the lower miniband could become exponentially low occupied and decoupled from the lower miniband states. At certain conditions, the $2Q$ lower-miniband states are mainly decoupled from the environment of the continuum of the excited states in the overall infinite-size Hilbert space and constitute a finite-size subspace of the Hilbert space of Q interacting qubits. The $2Q$ partial qubit states could be thought of as quasidegenerate single-condensate states which are not macroscopically occupied. The energy of atom interaction also can be adjusted (in particular, via a Feshbach resonance) so that the Bogoliubov couplings are spread over the entire lower miniband, but not above the energy gap.

The quantity of interest is the joint probability distribution of the occupations of any preselected subset of bare-particle excited states or groups of such states in the equilibrium phase specified by the macroscopic wave function of the entire-trap condensate appeared due to spontaneous symmetry breaking in the course of the BEC phase transition. This subset of states or groups of states should be variable and controllable by tuning each detector for occupation measurement projecting upon a prescribed state or group of states. For example, in the case of a 2D multiqubit trap one could use a multidetector imaging by light propagating through the trap perpendicular to its plane and detect separately an occupation of excited states localized in each single-qubit cell or any other cell from a system of cells chosen for multidetector imaging. Such a geometry allows one to easily reconfigure the system of cells for detection, that is, to collect joint-occupation statistics for different subsets of groups of states. The latter is necessary for revealing manifestations of computational complexity in the atomic boson sampling. Further comments on the boson-sampling testing in the BEC trap are given in Sec. VII.

III. QUASIPARTICLES VERSUS BEC-MODIFIED WAVE FUNCTIONS: BOGOLIUBOV TRANSFORM AND MULTIMODE SQUEEZING

Quantum transitions of particles between excited states are described by the operators $\hat{a}_k^\dagger$ and $\hat{a}_k$ which create and annihilate, respectively, a particle in a state with a wave function $\psi_k(\mathbf{r})$ in a mesoscopic trap of a finite volume V confining a dilute interacting gas of N particles in total by means of some external potential $U(\mathbf{r})$. Let us consider an equilibrium state (described by a density matrix $\hat{\rho}$) of such a Bose-Enstein-condensed gas with a well-formed macroscopic wave function $\psi_0(\mathbf{r})$ of the condensate at a temperature T well below a critical region. This N-body system can be accurately described by means of the Bogoliubov-Popov approximation [42,43,82] via a set of quasiparticles whose creation and annihilation operators $\hat{b}_j^\dagger$ and $\hat{b}_j$ are related to the particle ones via two representations of the excited-particle field operator, $\hat{\psi}_{\text{ex}}(\mathbf{r}) = \sum_{k\neq 0} \psi_k(\mathbf{r})\hat{a}_k = \sum_j (u_j(\mathbf{r})\hat{b}_j + v_j^*(\mathbf{r})\hat{b}_j^\dagger)$, and a symplectic matrix R of Bogoliubov transformation:

$$V_{\hat{a}} = R\, V_{\hat{b}},\ V_{\hat{a}} \equiv (.., \hat{a}_k^\dagger, \hat{a}_k, ..)^T,\ V_{\hat{b}} \equiv (.., \hat{b}_j^\dagger, \hat{b}_j, ..)^T. \quad (1)$$

The superscript T stands for a transpose operation. Hereinafter, the superscript star (*) means complex conjugation. The vectors $V_{\hat{a}}$ and $V_{\hat{b}}$ consist of the creation and annihilation operators of the particles and quasiparticles, respectively. The basis of orthonormal bare-particle wave functions $\{\psi_k(\mathbf{r})|\, k = 1, 2, \ldots\}$ can be chosen arbitrarily. For instance, it could accommodate the single-particle wave functions prescribed for projection by detectors measuring the excited-state occupations.

The condensate obeys the Gross-Pitaevskii equation:

$$\hat{\mathscr{L}}\psi_0 = 0; \quad \hat{\mathscr{L}} \equiv -\frac{\hbar^2\Delta}{2M} + U + g\langle N_0\rangle\psi_0^2 + 2gn_{\text{ex}} - \mu. \quad (2)$$

Here Δ is the three-dimensional Laplace operator, $g = 4\pi\hbar^2 a/m$ an interaction constant, m a particle mass, μ a chemical potential, $\langle N_0\rangle$ a mean number of particles in the condensate, and $n_{\text{ex}}(\mathbf{r}) = \langle\hat{\psi}_{\text{ex}}^\dagger(\mathbf{r})\hat{\psi}_{\text{ex}}(\mathbf{r})\rangle$ is a mean density profile of the excited particle fraction. The angles stand for a statistical averaging, $\langle\ldots\rangle = \text{Tr}\{\ldots\hat{\rho}\}$. The two-component quasiparticle wave function $\{u_j, v_j\}$ of an energy E_j obeys the Bogoliubov-de Gennes equations:

$$\hat{\mathscr{L}}u_j + g\langle N_0\rangle\psi_0^2(\mathbf{r})(u_j + v_j) = +E_j u_j,$$
$$\hat{\mathscr{L}}v_j + g\langle N_0\rangle\psi_0^2(\mathbf{r})(u_j + v_j) = -E_j v_j. \quad (3)$$

The wave functions are normalized to unity as follows: $\int_V |\psi_0|^2 d^3\mathbf{r} = 1$, $\int_V (|u_j|^2 - |v_j|^2) d^3\mathbf{r} = 1$; $j = 1, 2, \ldots$. For simplicity of formulas, we assume that all wave functions ψ_0, u_j, v_j [and f_k in Eq. (4) below] are real-valued.

We'll solve these equations and expand the quasiparticle wave functions via an appropriate basis of excited states orthogonal to the condensate wave function. In principle, one may start with an arbitrary complete set of such excited states and apply an *ad hoc* orthonormalization procedure [67]. There is a more convenient choice of such states, namely, as the solutions to a single-particle BEC-modified Schrödinger equation [34,83],

$$\hat{\mathscr{L}} f_k = \epsilon_k f_k, \tag{4}$$

in which the potential is modified by the condensate (obviously, $f_0 = \psi_0$). The set of orthonormal solutions $\{f_k(\mathbf{r}) | k = 1, 2, ...\}$ forms a complete basis in the single-particle Hilbert space of excited states. In the basis $\{f_k\}$, a two-component wave function $\{u, v\}$ can be written as a vector $\mathbf{w} = \{w_{r,k} | r = 1, 2;\ k = 1, 2, ...\}$ with components constituting the wave functions $u(\mathbf{r}) = \sum_{k\neq 0} w_{1,k} f_k(\mathbf{r})$, $v^*(\mathbf{r}) = \sum_{k\neq 0} w_{2,k} f_k(\mathbf{r})$ and enumerated by a double index $K = (r, k)$. The Nambu-type index r runs over two values 1 and 2. The index k enumerates positions of the above two-component blocks in the natural order of increasing index k. As a result, the Bogoliubov-de Gennes equations (3) acquire a standard form of an algebraic problem on the eigenvalues E_j and eigenvectors $\mathbf{w}_j$ of a certain (2×2)-block matrix $\mathbb{B} = (\mathbb{B}_{k,k'})$,

$$\mathbb{B}\mathbf{w}_j = E_j \mathbf{w}_j; \quad \mathbb{B}_{k,k'} = (\sigma_z + i\sigma_y)\Delta_{k,k'} + \epsilon_k \sigma_z \delta_{k,k'}. \tag{5}$$

The latter involves the overlapping integrals

$$\Delta_{k,k'} = g\langle N_0\rangle \int f_k(\mathbf{r})\, \psi_0^2(\mathbf{r})\, f_{k'}(\mathbf{r})\, d^3\mathbf{r}, \tag{6}$$

which determine the Bogoliubov coupling coefficients, and the 2×2 Pauli matrices

$$\sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{7}$$

The $\delta_{k,k'}$ is the Kronecker delta.

This mean-field approach accounts for interactions and is not reduced to just a modification of the excitation spectrum. Via nonlinear Gross-Pitaevskii and Bogoliubov–de Gennes equations, the bare particles (atoms) acquire Bogoliubov couplings, Eq. (6), and form the quasiparticles—superpositions of many bare particles. The eigenvectors (quasiparticles) $\mathbf{w}_j$ are no less important than their eigenvalues (excited energies) E_j, especially since in the experiments detectors count the real atoms (bare particles), not virtual energy eigenvectors (quasiparticles). This fact brings into the game an interplay between the interference and interactions of bare particles. This interplay is the ultimate cause for (i) a self-generation of squeezed states by a quantum many-body interacting system even in the equilibrium (thermal) state and (ii) an appearance of computational complexity in atomic boson sampling revealed in this paper.

The matrix R, that describes the Bogoliubov transformation Eq. (1), can be viewed as a product of two matrices:

$$R = \mathbb{U}\tilde{R}, \quad \mathbb{U} = \left(U_{r,k}^{r',k'}\right). \tag{8}$$

The matrix $\mathbb{U}$ describes the transformation between two bases of two-component Bogoliubov states $\{u_j, v_j\}$, namely, from the creation and annihilation operators $\{\hat{\tilde{a}}_k^\dagger, \hat{\tilde{a}}_k\}$ in the basis of the BEC-modified particle states $\{f_k | k = 1, 2, \ldots\}$ to the creation and annihilation operators $\{\hat{a}_k^\dagger, \hat{a}_k\}$ in the basis of the bare-particle excited states $\{\psi_k | k = 1, 2, \ldots\}$ chosen for measuring the occupation numbers $\hat{n}_k = \hat{a}_k^\dagger \hat{a}_k$. It is formed by the intertwining unitary matrix U and its complex conjugate U^*, where U is the matrix of the transformation between those two bases in the single-particle Hilbert space:

$$f_k = \sum_{k'\neq 0} U_{k',k} \psi_{k'}. \tag{9}$$

In Eqs. (8) like in Eq. (23) for G, we enumerate the entries of the matrices, associated with both creation, $\hat{a}_k^\dagger$, and annihilation, $\hat{a}_k$, operators, by the double indices $K = (r, k)$ for rows and $K' = (r', k')$ for columns. The indices $k = 1, 2, \ldots$ and $k' = 1, 2\ldots$ stand for the position (row and column) of an entire 2×2 block. The dual indices $r = 1, 2$ and $r' = 1, 2$ specify the position (row and column) of the entry (such as $U_{r,k}^{r',k'}$) within that 2×2 block. The rows and columns are ordered in the natural order of increasing indices k and k' for the 2×2 blocks and increasing indices $r = 1, 2$ and $r' = 1, 2$ inside each 2×2 block. In terms of such a Nambu-type notation, we have $U_{1,k}^{1,k'} = (U^*)_{k,k'}$, $U_{2,k}^{2,k'} = U_{k,k'}$, $U_{2,k}^{1,k'} = U_{1,k}^{2,k'} = 0$.

The matrix $\tilde{R}$ stands for the specific Bogoliubov transformation (1) that relates the quasiparticle creation and annihilation operators $\hat{b}_k^\dagger, \hat{b}_k$ to the creation and annihilation operators $\hat{\tilde{a}}_k^\dagger, \hat{\tilde{a}}_k$ associated with the BEC-modified particles defined by Eq. (4); $\hat{\psi}_{\rm ex}(\mathbf{r}) = \sum_{k\neq 0} f_k(\mathbf{r})\hat{\tilde{a}}_k$. The Bogoliubov matrix $\tilde{R}$ diagonalizes the Bogoliubov–de Gennes matrix $\mathbb{B}$ in Eqs. (5):

$$\tilde{R}^{-1}\mathbb{B}\tilde{R} = \bigoplus_j E_j \sigma_z, \quad \tilde{R} = \left(\tilde{R}_{r,k}^{r',k'}\right). \tag{10}$$

The matrix $\tilde{R}$ is a (2×2)-block matrix whose 2×2 entry for the given block indices k, k',

$$\left(\tilde{R}_{r,k}^{r',k'}\right) = \left(P_{k,k'}\begin{bmatrix} \cosh \xi_{k,k'} & \sinh \xi_{k,k'} \\ \sinh \xi_{k,k'} & \cosh \xi_{k,k'} \end{bmatrix}\right), \tag{11}$$

is the product of the Lorentzian 2×2 matrix containing the relative partial squeezing parameter $\xi_{k,k'}$, given by the energies $E_{k'}, \epsilon_k$ as follows:

$$\cosh \xi_{k,k'} = \frac{\epsilon_k + E_{k'}}{2\sqrt{\epsilon_k E_{k'}}}, \quad \sinh \xi_{k,k'} = \frac{\epsilon_k - E_{k'}}{2\sqrt{\epsilon_k E_{k'}}}, \tag{12}$$

and the factor $P_{k,k'}$ accounting for a mixing weight of the BEC-modified excited wave function $f_{k'}$ in the expansion of the k-quasiparticle two-component wave function:

$$u_{k'}(\mathbf{r}) = \sum_{k\neq 0} (\cosh \xi_{k,k'}) P_{k,k'} f_k(\mathbf{r}),$$

$$v_{k'}(\mathbf{r}) = \sum_{k\neq 0} (\sinh \xi_{k,k'}) P_{k,k'} f_k(\mathbf{r}). \tag{13}$$

The matrix $P = (P_{k,k'})$ is unitary (in fact, orthogonal) since the Bogoliubov transformation (1) is symplectic, that is, keeps invariant the canonical Bose commutation relations for the creation and annihilation operators. The intersection of the odd rows and odd columns of $\tilde{R}$ as well as the intersection of the even rows and even columns of $\tilde{R}$ form the same submatrix, while the intersection of the odd rows and even columns of $\tilde{R}$ as well as the intersection of the even rows and odd columns of $\tilde{R}$ form the other same submatrix:

$$\tilde{R}_1^1 = \tilde{R}_2^2 = \big(\tilde{R}_{1,k}^{1,k'}\big) = \big(\tilde{R}_{2,k}^{2,k'}\big) = (P_{k,k'}\cosh\xi_{k,k'}),$$
$$\tilde{R}_1^2 = \tilde{R}_2^1 = \big(\tilde{R}_{1,k}^{2,k'}\big) = \big(\tilde{R}_{2,k}^{1,k'}\big) = (P_{k,k'}\sinh\xi_{k,k'}). \quad (14)$$

Both nonvanishing off-diagonal entries $\xi_{k,k'}$ and $P_{k,k'}$ at $k \neq k'$ are responsible for the multimode squeezing in the system of atomic modes associated with the BEC-modified excited states. The quasiparticles define the eigenenergy modes which are completely independent of each other, are not squeezed, and stay in a thermal state when in equilibrium. On the contrary, the BEC-modified excited states correspond to the excited modes which form a mutually squeezed multimode system due to mixing via the unitary matrix P.

In terms of a column vector composed of all the creation operators in its upper half and all the annihilation operators in its lower half, that is not in the alternating pattern of Eq. (1), the matrix $\tilde{R}$ performs the following Bogoliubov transformation:

$$\begin{pmatrix}\hat{\mathbf{a}}^\dagger\\ \hat{\mathbf{a}}\end{pmatrix} = \begin{bmatrix}\tilde{R}_1^1 & \tilde{R}_1^2\\ \tilde{R}_2^1 & \tilde{R}_2^2\end{bmatrix}\begin{pmatrix}\hat{\mathbf{b}}^\dagger\\ \hat{\mathbf{b}}\end{pmatrix}. \quad (15)$$

Here $\hat{\mathbf{b}}^\dagger = (\hat{b}_1^\dagger, \hat{b}_2^\dagger, \dots)^T$ and $\hat{\mathbf{b}} = (\hat{b}_1, \hat{b}_2, \dots)^T$ as well as alike boldface operator vectors are the column vectors of the creation and annihilation operators, respectively.

The Bogoliubov transformation $\tilde{R}$ can be concisely described via the polar decomposition of its blocks (14) into a product of a unitary matrix and a Hermitian matrix:

$$(P_{k,k'}\cosh\xi_{k,k'}) = \mathcal{P}\cosh r,$$
$$(P_{k,k'}\sinh\xi_{k,k'}) = \mathcal{P}e^{i\theta}\sinh r. \quad (16)$$

So, we have a product of a polar part, represented by unitary matrices $\mathcal{P}$ or $\mathcal{P}e^{i\theta}$, and a Hermitian part, represented by the hyperbolic functions cosh r or sinh r of the multimode squeezing matrix r. The matrix r is a positive semidefinite Hermitian matrix. The matrices cosh r, $\mathcal{P}$, and $\mathcal{P}e^{i\theta}$ are given by the following explicit formulas:

$$\cosh r = [(P_{k,k'}\cosh\xi_{k,k'})^T(P_{k,k'}\cosh\xi_{k,k'})]^{1/2},$$
$$\mathcal{P} = (P_{k,k'}\cosh\xi_{k,k'})(\cosh r)^{-1},$$
$$\mathcal{P}e^{i\theta} = (P_{k,k'}\sinh\xi_{k,k'})(\sinh r)^{-1}. \quad (17)$$

Note that the matrices $\mathcal{P}$ and P are not the same. Thus, the Bogoliubov transformation (8) is a superposition

$$\begin{pmatrix}\hat{\mathbf{a}}^\dagger\\ \hat{\mathbf{a}}\end{pmatrix} = \begin{bmatrix}(U\mathcal{P})^* & 0\\ 0 & U\mathcal{P}\end{bmatrix}\begin{bmatrix}\cosh r & (e^{i\theta}\sinh r)^*\\ e^{i\theta}\sinh r & \cosh r^*\end{bmatrix}\begin{pmatrix}\hat{\mathbf{b}}^\dagger\\ \hat{\mathbf{b}}\end{pmatrix} \quad (18)$$

of a transformation, specified by the Hermitian matrix of squeezing parameters $r = (r_{k,k'})$ and the unitary $e^{i\theta}$, and a unitary transformation, which is the product of two block-diagonal unitary transformations specified by the unitary $\mathcal{P}$ and an arbitrary unitary U. The unitary $\mathcal{P}$ is associated with the transformation from the quasiparticles to the BEC-modified excited states $\{f_k\}$, while the unitary U describes a further transformation from the wave-function basis $\{f_k\}$ to any basis of excited states $\{\psi_k\}$ chosen for projection upon by detectors measuring occupations of excited states or groups of them.

For comparison with Gaussian boson sampling in the optical interferometer, one can represent the Bogoliubov transformation (18) via the quantum optics formalism (see Refs. [84–89] and references therein), namely, as a unitary evolution, governed by a unitary multimode squeeze operator

$$\hat{S} = \exp\left[\frac{\hat{\mathbf{b}}^{\dagger\mathbf{T}}S\hat{\mathbf{b}}^\dagger - \hat{\mathbf{b}}^{\mathbf{T}}S^\dagger\hat{\mathbf{b}}}{2}\right]; \quad S = e^{i\theta}r = r^*e^{i\theta^*}, \quad (19)$$

and a unitary multimode rotation operator

$$\hat{\Phi} = \exp(i\hat{\mathbf{b}}^{\dagger\mathbf{T}}\Phi\hat{\mathbf{b}}), \quad \Phi = \Phi^\dagger, \quad (20)$$

with an additional excited-state transformation described by a unitary matrix U like the one in Eqs. (8):

$$\hat{\mathbf{a}}^\dagger = U^*\hat{S}^\dagger\hat{\Phi}^\dagger\hat{\mathbf{b}}^\dagger\hat{\Phi}\hat{S}$$
$$= U^*e^{-i\Phi^*}(\cosh r)\hat{\mathbf{b}}^\dagger + U^*e^{i\Phi}e^{-i\theta^*}(\sinh r^*)\hat{\mathbf{b}},$$
$$\hat{\mathbf{a}} = U\hat{S}^\dagger\hat{\Phi}^\dagger\hat{\mathbf{b}}\hat{\Phi}\hat{S}$$
$$= Ue^{-i\Phi^*}e^{i\theta}(\sinh r)\hat{\mathbf{b}}^\dagger + Ue^{i\Phi}(\cosh r^*)\hat{\mathbf{b}}. \quad (21)$$

A symmetric matrix S defining the squeeze operator is represented via two Hermitian matrices r and θ. A Hermitian matrix Φ defines the rotation operator $\hat{\Phi}$. A size of vectors and matrices is determined by a number M of modes in the system.

Clearly, the Bogoliubov transformation (21) matches the one in Eq. (18) when one sets $S = e^{i\theta}r$, $e^{i\Phi} = \mathcal{P}$, so $e^{i\Phi}\cosh r^* = \tilde{R}_2^2$ and $e^{-i\Phi^*}e^{i\theta}\sinh r = \tilde{R}_2^1$.

We conclude that the values of the inter- and intramode squeezing, defined by the squeezing parameters $r_{k,k'}$ (that is, in essence, by the entries of the matrices r or cosh r or sinh r) is determined by the Hadamard (that is, entry by entry, not standard, row by column) product of matrices $(P_{k,k'})$ and $(\cosh\xi_{k,k'})$ or $(\sinh\xi_{k,k'})$ in Eq. (14). If it was the standard matrix product, then the intermode mixing via the unitary mixing matrix P would play a part of a unitary matrix U and the strength of the multimode squeezing would be determined just by the Lorenzian partial squeezing parameters $\xi_{k,k'}$ in Eqs. (12). However, in reality, the effect of the interparticle interaction turned by the inhomogeneous condensate into the overlapping integrals (6) (i.e., Bogoliubov couplings) is not as simple as the latter scenario may suggest. The point is that the two effects, the effect of a direct squeezing of a partial k-mode induced by a quasiparticle k' mode via the off-diagonal coefficient $\xi_{k,k'}$ and the effect of a unitary mixing of a partial k mode with a quasiparticle k' mode given by the off-diagonal coefficient $P_{k,k'}$ do not contribute to the Bogoliubov transformation independently via just the standard product of two matrices. On the contrary, the contributions of those two effects nontrivially intertwine since the combined effect is given by the Hadamard product of the matrices $(P_{k,k'})$ and $(\cosh\xi_{k,k'})$ or $(\sinh\xi_{k,k'})$.

IV. JOINT PROBABILITY DISTRIBUTION OF THE EXCITED PARTICLE OCCUPATIONS VIA THE CHARACTERISTIC FUNCTION, THE HAFNIAN MASTER THEOREM

Consider occupations of any basis states $\{\psi_k | k \neq 0\}$ in the single-particle Hilbert space. They are described by the Hermitian operators $\hat{n}_k = \hat{a}_k^\dagger \hat{a}_k$ and can be measured by the appropriate detectors projecting particles onto these states. We calculate the joint probability distribution $\rho(\{n_k\})$ of these observables $\{\hat{n}_k | k \neq 0\}$ by means of the well-known approach of the characteristic function $\Theta(\{u_k\})$ and cumulant expansion (see, for example, Refs. [90–93] and references therein) as follows:

$$\rho(\{n_k\}) = \int_{-\pi}^{\pi} ... \int_{-\pi}^{\pi} e^{-i\sum_k u_k n_k} \Theta(\{u_k\}) \prod_k \frac{du_k}{2\pi},$$
$$\Theta(\{u_k\}) = \langle e^{i\sum_k u_k \hat{n}_k} \rangle \equiv \mathrm{Tr}\{e^{i\sum_k u_k \hat{n}_k} \hat{\rho}\}. \quad (22)$$

Utilizing the method employed in Ref. [34] but assigning now an individual argument $z_k = e^{iu_k}$ to each excited state, we get the characteristic function of this distribution:

$$\Theta = \frac{1}{\sqrt{\det[\mathbb{1} - (Z - \mathbb{1})G]}}, \quad G_{r,k}^{r',k'} = \langle : \hat{a}_{r,k}^\dagger \hat{a}_{r',k'} : \rangle. \quad (23)$$

[See Appendices A and B for details on the derivation of Eqs. (23) and (24) for the joint occupation probability distribution of the excited particle states and the Hafnian master theorem (28).] Here G is the covariance matrix with entries $G_K^{K'}$, enumerated by double indices $K = (r, k)$ for rows and $K' = (r', k')$ for columns and equal to normally ordered (note colons) averages of a product of two creation or annihilation operators. Nambu-type index r acquires two values: 1, 2. For any operator $\hat{\mathcal{O}}$, it denotes that same operator, $\hat{\mathcal{O}}_r = \hat{\mathcal{O}}$, if $r = 1$ or its Hermitian conjugate, $\hat{\mathcal{O}}_r = \hat{\mathcal{O}}^\dagger$, if $r = 2$. It is related to the (2×2)-block structure of the matrix. The identity matrix is denoted by the symbol $\mathbb{1}$.

The variables form a diagonal matrix $Z = \mathrm{diag}(\{z_K\})$ which contains pairs of the same variable $z_{r,k} = z_k = e^{iu_k}$ along the diagonal and has a size that is twice the number M of excited particle states in the considered miniband.

The result (23) is truly general and universal since it gives the statistics of the joint occupations of any restricted, marginal number of states M or coarse-grained groups of states by any number of the interacting noncondensed atoms $N - \langle N_0 \rangle$.

Its derivation via quasiparticles entails the covariance matrix expressed via the symplectic Bogoliubov matrix R as follows:

$$G = RDR^\dagger + \frac{RR^\dagger - \mathbb{1}}{2}. \quad (24)$$

Here the (2×2)-block diagonal matrix D is determined by thermal population of the quasiparticle excitations:

$$D = \bigoplus_j \frac{1}{e^{E_j/T} - 1} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}. \quad (25)$$

We derived Eq. (23) also within the microscopic theory of critical phenomena [45–47] via the method of the recurrence equations for the partial operator contractions, unrelated to the Bogoliubov-Popov picture of the BEC-condensed gas. It is valid for any system of the interacting unconstraint bosons in an equilibrium state described by any normally ordered covariance matrix G, that is, for any state $\hat{\rho} = e^{-\hat{H}/T}/\mathrm{Tr}\{e^{-\hat{H}/T}\}$.

The joint occupation probability distribution is given by the mixed derivatives:

$$\rho(\{n_k\}) = \prod_k \frac{\partial^{n_k}}{n_k! \, \partial z_k^{n_k}} \Theta \Big|_{\{z_k = 0\}}, \quad \{z_k \equiv e^{iu_k} | k = 1, 2, ...\}. \quad (26)$$

We get the distribution (26) explicitly as follows:

$$\rho(\{n_k\}) = \frac{\mathrm{haf}\tilde{C}(\{n_k\})}{\sqrt{\det(\mathbb{1} + G)} \prod_k n_k!}, \quad C = AG(\mathbb{1} + G)^{-1}, \quad (27)$$

where the permutation matrix $A = \bigoplus_j \sigma_x$ contains the Pauli matrix σ_x and makes the matrices C and $\tilde{C}(\{n_k\})$ under the Hafnian symmetric. We derive Eq. (26) from Eq. (23) via the Wick's theorem, which is well-known in the quantum field theory [94,95] and is equivalent, in this case, to the Hafnian master theorem (Appendix B):

$$\frac{1}{\sqrt{\det(\mathbb{1} + (\mathbb{1} - Z)G)}} = \sum_{\{n_k\}} \frac{\mathrm{haf}\tilde{C}(\{n_k\})}{\sqrt{\det(\mathbb{1} + G)}} \prod_k \frac{z_k^{n_k}}{n_k!}. \quad (28)$$

In fact, the Hafnian [37,96] was introduced in Refs. [97,98] as a notation for a Wick's sum of all possible products of n two-operator contractions (averages) in a given product of $2n$ creation or annihilation operators. Here the Hafnian is a function of the $(2n\times2n)$-matrix $\tilde{C}(\{n_k\})$, $n = \sum_k n_k$, built from the matrix C, Eq. (27), via replacing the kth pair of rows with the n_k copies of the kth pair of rows for all $k = 1, ..., M$ and then replacing the k'th pair of columns in the $(n\times2M)$-matrix, obtained at the first step, with the $n_{k'}$ copies of the k'th pair of columns for all $k' = 1, \dots, M$. The MacMahon master theorem (30) follows from (28) as a particular case. The very definition of the Hafnian as a sum of the products of just n entries of a $(2n\times2n)$-matrix $\tilde{C}$, $\mathrm{haf}\tilde{C} = \frac{1}{2^n n!} \sum_{\sigma \in S_{2n}} \prod_{j=1}^{n} \tilde{C}_{\sigma(2j-1)}^{\sigma(2j)}$, is designed to account properly for the (2×2)-block structure of the matrices C and $\tilde{C}$. The latter also inherits the (2×2)-block structure of the matrix Z that corresponds to the derivatives of the determinantal function $1/\sqrt{\det(\mathbb{1} - ZC)}$ over pairs of equal variable $z_k = z_{1,k} = z_{2,k}$ in each (2×2)-block of the diagonal matrix Z at the point $\{z_k = 0\}$. The definitions of the permanent, $\mathrm{per}\tilde{C} = \sum_{\sigma \in S_{2n}} \prod_{i=1}^{2n} \tilde{C}_i^{\sigma(i)}$, and the determinant, $\det \tilde{C} = \sum_{\sigma \in S_{2n}} \mathrm{sgn}(\sigma) \prod_{i=1}^{2n} \tilde{C}_i^{\sigma(i)}$, have nothing to do with the (2×2)-block structure of the matrices. In the above formulas, S_{2n} is the symmetric group of all $(2n)!$ permutations of the set $\{1, 2, ..., 2n\}$. At the origin of the coordinate system $\{z_k = 0\}$, the square root on the left-hand side of Eq. (28) is $\sqrt{\det(\mathbb{1} + (\mathbb{1} - Z)G)}|_{\{z_k=0\}} = \sqrt{\det(\mathbb{1} + G)}$ and, accordingly, we assume that $\mathrm{haf}\tilde{S}(\{n_k = 0 | k = 1, \dots, M\}) = 1$ on the right-hand side of Eq. (28).

The distribution (27) was also derived via a standard phase-space method [99,100] and applied to the photon sampling of Gaussian states in Refs. [19,20]. The phase-space method had been applied in BEC statistics in Ref. [101] for rederiving an original result of [33] on the statistics of a Gaussian state of atomic modes squeezed by Bogoliubov coupling. In Appendix A, we use the method of Ref. [101].

Remarkably, the result (23) for the characteristic function is universal in the sense that it has the same universal form for any marginal restricted subset of the excited particle states or coarse-grained groups of excited states, if one considers them irrespective to the other states. Averaging over the rest of the excited-state occupations is achieved by setting all irrelevant variables $z_{k'}$ equal to zero and keeping just those rows and columns in the matrices A, D, G, C which are associated with the chosen marginal subset of excited states. Combining some excited states into a coarse-grained group is accomplished in Eqs. (23) and (28) by setting equal all of the variables $\{z_k\}$ within such a group. If the characteristic function was not universal in this sense, then one would need to rederive the formula for it from scratch for any new preselected subset or coarse-grained groups of excited states.

V. CUMULANT ANALYSIS

Here we point out that the cumulant analysis and the result for the characteristic function (23) provide the most efficient, canonical method for characterizing such a complex joint distribution and distinguishing it from various mockups via generating cumulants [33] $\{\tilde{\kappa}_{\{m_k\}}|m_k = 1, 2, ...\}$ defined by the Taylor expansion

$$\ln\Theta = \sum_{\{m_k\}} \tilde{\kappa}_{\{m_k\}} \prod_k \frac{(e^{iu_k}-1)^{m_k}}{m_k!} \tag{29}$$

and directly related to the moments and cumulants of the distribution.

One could use the permanent master theorem,

$$\frac{1}{\det(\mathbb{1}-ZC)} = \sum_{\{s_K\}} \left[\text{per}\, C(\{s_K\}) \prod_K \frac{z_K^{s_K}}{s_K!} \right], \tag{30}$$

of MacMahon [35,36]. A double index $K = (r, k)$ runs over all rows of a matrix $C(\{s_K\})$; $\{s_K\}$ is a set of non-negative integers. It is valid for any, even not pairwise equal variables $z_{1,k}, z_{2,k}$. The coefficients of this Taylor expansion are given by the permanent of the $C(\{s_K\})$ which is the C with the Kth row and Kth column replaced by the same Kth row and Kth column s_K times.

If we had $2M$ stochastic variables, i.e., the number $2M$ of independent variables z_K in the matrix Z was equal to the number of matrix rows, and the square root in Eq. (23) for the characteristic function was absent, then we would at once conclude that the occupation probability,

$$\rho'(\{s_K\}) = \frac{\text{per}\,(C(\{s_K\}))}{\det(\mathbb{1}+G)\prod_K s_K!}, \quad C = AG(\mathbb{1}+G)^{-1}, \tag{31}$$

is given by a permanent of the extended matrix $C(\{s_K\})$ built of the matrix C as stated above. The characteristic function Θ' of such an auxiliary probability distribution has an extended set of the generating cumulants $\tilde{\kappa}'_{\{m_K\}}$:

$$\ln\Theta' = \sum_{\{m_{r,k}\}} \tilde{\kappa}'_{\{m_{r,k}\}} \prod_{r,k} \frac{(e^{iu_{r,k}}-1)^{m_{r,k}}}{m_{r,k}!}. \tag{32}$$

Since in Eq. (23) (a) there are two times less independent variables because $z_{1,k} = z_{2,k} = z_k$ and (b) the square root adds a prefactor $1/2$ for $\ln\Theta$, we get the true generating cumulants as the simple finite sums of the auxiliary ones:

$$\tilde{\kappa}_{\{m_k\}} = \frac{1}{2}\sum_k \sum_{m_{1,k}=0}^{m_k} \left[\tilde{\kappa}'_{\{m_{1,k}, m_k - m_{1,k}\}} \prod_{k'} \binom{m_{1,k'}}{m_{k'}} \right]. \tag{33}$$

Here a pair of the arguments $m_{r,k}$, $r = 1, 2$, in $\tilde{\kappa}'_{\{m_{r,k}\}}$ is written explicitly for the case when $m_{1,k} + m_{2,k} = m_k$; $\binom{m_{1,k}}{m_k} = m_k!/(m_{1,k}!m_{2,k}!)$ is a binomial coefficient. Thus, we obtain an implicit characterization of the joint occupation probability distribution of the excited particle states via the cumulants in Eq. (33) and the permanents in Eq. (31). However, the permanent master theorem of MacMahon does not directly provide an explicit analytical formula for the distribution (26) via permanents.

Remarkably, computing the cumulants and joint probability distribution for the excited particle occupations is a $\sharp P$-hard problem. This is related to a $\sharp P$-hard complexity of computing the permanents [38] and the fact that the (2×2)-block structure of the matrices A, D, G, C and the presence of the square root in Eq. (23) [the prefactor $1/2$ in Eq. (33)] just modify it a bit to a similar, Hafnian ♯P-hard complexity, Eq. (27). Note also that computing a cumulant amounts to computing an infinite sum of permanents or Hafnians which is similar to a sum representing a torontonian. Such a sum is known to be ♯P-hard for computing [22].

To show a ♯P-hardness of cumulant computing, let us first consider the generating cumulants $\tilde{\kappa}_{\{n_k\}}$, Eq. (29). They are very similar to the probabilities $\rho(\{n_k\})$, Eqs. (23) and (26), since they are the coefficients in the Taylor expansion of the logarithm of the characteristic function over the variables $\{z_k - 1\}$ and the characteristic function over the variables $\{z_k\}$,

$$\ln\Theta = \sum_{\{n_k\}} \tilde{\kappa}_{\{n_k\}} \prod_k \frac{(z_k-1)^{n_k}}{n_k!}, \tag{34}$$

$$\Theta = \sum_{\{n_k\}} \rho(\{n_k\}) \prod_k z_k^{n_k}, \tag{35}$$

respectively. Both the characteristic function and its logarithm are well-behaved, nonsingular analytic functions in the vicinity of the origin of coordinate system $\{z_k = 0\}$ where the characteristic function equals unity and its logarithm equals zero. In essence, the logarithm just smoothly modifies the characteristic function, and a uniform shift of all variables z_k by unity, $z_k \to z_k - 1$, just regroups the coefficients in the Taylor expansion. The latter shift means representing the matrix Z in Eq. (28) as $Z = (Z - \mathbb{1}) + \mathbb{1}$ that amounts to just rescaling the matrix $C = AG(\mathbb{1}+G)^{-1}$ to the new matrix $C = AG$, which now defines the matrix $\tilde{C}(\{n_k\})$ under the Hafnians in the Taylor expansion over the shifted variables $z_k - 1$, while the Hafnians and their ♯P-hard complexity, of course, do not disappear. As a result, the generating cumulants are as ♯P-hard for computing as the probabilities, that is, the Hafnians in Eq. (27).

Finally, the standard cumulants $\kappa_{\{n_k\}}$, that is, the coefficients in the Taylor expansion of the logarithm of the characteristic function over the variables $u_k = -i \ln(z_k)$,

$$\ln \Theta = \sum_{\{n_k\}} \kappa_{\{n_k\}} \prod_k \frac{(iu_k)^{n_k}}{n_k!}, \quad (36)$$

are just finite linear combinations of the generating cumulants $\tilde{\kappa}_{\{n_k\}}$ of orders up to $\{n_k\}$ with the coefficients a la Stirling numbers of the second kind [33]. Thus, computing the standard cumulants is also ♯P-hard.

VI. FURTHER COMMENTS ON THE ♯P-HARDNESS OF ATOMIC BOSON SAMPLING

Fortunately, the ♯P-hardness analysis of the average and approximate cases for the atomic and photonic boson samplings are very similar since the universal result in Eqs. (23) and (27) puts these two samplings on the same footing, both with respect to expressing the joint probability via the Hafnian and ranging complex-valued matrices associated with the sampling. For the interferometer, a wide range of complex unitary matrices appears due to varying its partial modes via adjusting phase shifts and couplings. For the BEC, a wide range of complex matrices appears due to varying the partial atomic wave functions (excited states) assigned to be projected upon for detectors measuring their occupations. In particular, the "hiding" technique employed in quantum optics works equally well for both samplings. Besides, in both samplings, the squeezing parameters of the matrix under the Hafnian are controllable via adjusting squeezing in the input sources in the optical interferometer or the condensate wave function and Bogoliubov couplings (6) by changing the trapping potential, interaction (via Feshbach resonances [102]), temperature, or number of trapped atoms. We skip repeating such ♯P-hardness analyses, see Refs. [2,11,15,20–22,26,32,103–107].

We just point to the Haar randomness of unitary matrices, which essentially determines an entire set and range of variable parameters available in both quantum sampling systems—the linear interferometer and the BEC trap. The point is that the covariance matrix G, entering the characteristic function in Eq. (23) and the occupation probabilities in Eq. (28), depends on the unitary matrix U [Eqs. (8)] that describes a transformation from the basis of the solutions $\{f_k|\, k = 1, 2, \ldots\}$ of the BEC-modified Schrodinger equation (4) to a variable basis of the bare-particle excited states $\{\psi_k|\, k = 1, 2, \ldots\}$ chosen for projection upon when measuring the excited-state occupations by multidetector imaging, Eq. (9). This dependence occurs via Eq. (24) for G since it involves the symplectic Bogoliubov matrix R. Then, the ♯P-hardness follows from the usual argument [2,19,20] based on the fact that the Haar randomness of the unitary matrices essentially yields the Gaussian randomness of the $\tilde{C}(\{n_k\})$ matrices. The ♯P-hardness of computing the permanent or Hafnian of a random Gaussian matrix is well-known.

Moreover, the atomic boson sampling in the BEC trap possesses a functional variability provided by a possibility to control the trapping potential as a function of spatial coordinates. In principle, it allows one to control all of the entries of the Bogoliubov coupling matrix (6), that is, also the extra $M(M-1)/2$ mutual intermode squeezing parameters $r_{k,k'}$, Eq. (18), not just M intramode squeezing parameters for each mode. In the Gaussian boson sampling in the linear interferometer, the squeezing is provided only to each mode separately at the input ports of the interferometer by means of the external sources of squeezed photons. Such a Gaussian boson sampling is analogous to a very special case of atomic boson sampling in a degenerate trap when the matrix $(r_{k,k'})$ of squeezing parameters reduces to a quasidiagonal matrix. The latter occurs, for example, when only a single-mode or two-mode Bogoliubov coupling and, hence, squeezing are present, like in a box trap with a uniform potential. The photon sources capable of providing and controlling all of the $M(M-1)/2$ mutual intermode squeezings are not available.

The presence of those additional off-diagonal squeezing parameters $r_{k,k'}$ makes the atomic boson sampling in a BEC trap with a multimode Bogoliubov coupling (6) more liable to ♯P-hardness than Gaussian boson sampling in the linear interferometer.

Such an additional randomness due to the off-diagonal squeezing parameters $r_{k,k'}$ can be converted into a randomness due to an extra unitary matrix V appearing on the right-hand side of the polar decomposition (16),

$$(P_{k,k'} \cosh \xi_{k,k'}) = \mathcal{P} V (\cosh\, \Lambda_r) V^\dagger, \quad (37)$$

if we replace the matrix r by its diagonal representation:

$$r = V \Lambda_r V^\dagger; \quad r\mathbf{v}_j = r_j \mathbf{v}_j, \quad \Lambda_r = \mathrm{diag}\{r_j|\, j = 1, \ldots, M\}. \quad (38)$$

The singular value decomposition in Eq. (37) is based on the singular vectors $\{\mathbf{v_j}|\, j = 1, \ldots, M\}$ and singular values $r_j \geqslant 0$, which are the eigenvectors (comprising the unitary V as columns) and the eigenvalues (comprising the diagonalized squeezing matrix Λ_r) of the squeezing matrix r, respectively. A singular vector $\mathbf{v}_j$ can be viewed as a column of complex amplitudes of the excited states in a jth eigen-squeezed mode that has the single-mode squeezing parameter r_j and is not subject to an intermode squeezing with other eigen-squeezed modes, $r_{j,j'} = 0\ \forall j' \neq j$. The result is the following Bloch-Messiah reduction [85,86] of the Bogoliubov transformation (18),

$$\begin{pmatrix} \hat{\mathbf{a}}^\dagger \\ \hat{\mathbf{a}} \end{pmatrix} = \begin{bmatrix} W^* & 0 \\ 0 & W \end{bmatrix} \begin{bmatrix} \cosh\, \Lambda_r & \sinh\, \Lambda_r \\ \sinh\, \Lambda_r & \cosh\, \Lambda_r \end{bmatrix} \begin{bmatrix} V^T & 0 \\ 0 & V^\dagger \end{bmatrix} \begin{pmatrix} \hat{\mathbf{b}}^\dagger \\ \hat{\mathbf{b}} \end{pmatrix}, \quad (39)$$

where the unitaries W and V are chosen to satisfy the so-called rotation condition emphasized in Ref. [86] in view of a possible nonuniqueness of the singular value decomposition, particularly in the presence of degenerate singular values. Equation (39) describes the overall Bogoliubov transformation as a parallel single-mode squeezing in all the eigen-squeezed modes preceded by some unitary mode mixing and followed by a different unitary mode mixing.

Taking advantage of this unique Bloch-Messiah representation, unambiguously specified by the preferred basis of quasiparticle states diagonalizing the Bogoliubov Hamiltonian and the preferred basis of the eigen-squeezed single-particle excited states diagonalizing the squeezing matrix, we obtain the normally ordered covariance matrix (24) in the following canonical form:

$$\bar{G} = \begin{bmatrix} W^* & 0 \\ 0 & W \end{bmatrix} (\bar{G}_Q + \bar{G}_T) \begin{bmatrix} W^T & 0 \\ 0 & W^\dagger \end{bmatrix}, \quad (40)$$

where

$$\bar{G} \equiv \begin{bmatrix} G_1^1 & G_1^2 \\ G_2^1 & G_2^2 \end{bmatrix} = \mathbb{A}^T G \mathbb{A}, \quad \mathbb{A} = (\delta_{i,2j-1-(2M-1)\theta(j-M)}).$$

Here, similar to Eq. (39) and contrary to the Nambu-type enumeration adopted in (23), we use the permutation $2M \times 2M$ matrix $\mathbb{A}$ (defined above via the Kronecker delta and the step function $\theta(x) = 1$ if $x > 0, \theta(x) = 0$ if $x \leqslant 0$) to convert the matrix G in Eq. (23) into the matrix $\bar{G}$ with the following block enumeration of rows and columns: The upper half of rows includes all correlations $\langle : \hat{a}^\dagger{}_{1,k} \hat{a}_{r',k'} : \rangle$ containing a creation operator at the left position, while the lower half of rows includes all correlations $\langle : \hat{a}^\dagger{}_{2,k} \hat{a}_{r',k'} : \rangle$ containing an annihilation operator at the left position. The first half of columns includes all correlations $\langle : \hat{a}^\dagger{}_{r,k} \hat{a}_{2,k'} : \rangle$ containing a creation operator at the right position, while the second half of columns includes all correlations $\langle : \hat{a}^\dagger{}_{r,k} \hat{a}_{1,k'} : \rangle$ containing an annihilation operator at the right position. A matrix with such a block enumeration of rows and columns is denoted by a bar above the symbol of a matrix.

The irreducible covariance matrices $\bar{G}_Q$ and $\bar{G}_T$,

$$\bar{G}_Q = \frac{RR^\dagger - 1}{2} = \begin{bmatrix} \sinh^2 \Lambda_r & \sinh \Lambda_r \cosh \Lambda_r \\ \sinh \Lambda_r \cosh \Lambda_r & \sinh^2 \Lambda_r \end{bmatrix}, \quad (41)$$

$$\bar{G}_T = RDR^\dagger = \begin{bmatrix} \cosh \Lambda_r & \sinh \Lambda_r \\ \sinh \Lambda_r & \cosh \Lambda_r \end{bmatrix} \begin{bmatrix} q^* & 0 \\ 0 & q \end{bmatrix} \begin{bmatrix} \cosh \Lambda_r & \sinh \Lambda_r \\ \sinh \Lambda_r & \cosh \Lambda_r \end{bmatrix}, \quad (42)$$

stand for the pure quantum (that is, at zero temperature, $T = 0$) and complimentary thermal (at $T \neq 0$) contributions to the total covariance matrix $\bar{G} = \bar{G}_Q + \bar{G}_T$, respectively, and are written in the basis of the eigen-squeezed single-particle excited states $\{\mathbf{v_j} | j = 1, ..., M\}$; $q = V^\dagger \operatorname{diag}\{(e^{E_j/T} - 1)^{-1} | j = 1, \dots, M\} V$. The block diagonal matrices in Eq. (39), built of the unitary matrix W and its inverse matrix $W^{-1} = W^\dagger$, describe the pure unitary forward and backward transformations between an arbitrary bare-particle basis and the eigen-squeezed basis of excited states in the single-particle Hilbert space.

The Bloch-Messiah reduction has been used in Refs. [88,89] for discussion of a hierarchy of various Gaussian boson samplings with photon sources at zero and finite temperatures. A general case has been named vibronic boson sampling since a modern discussion of Gaussian boson sampling is an extension of the previous detailed analysis [108] of vibronic transitions in polyatomic molecules.

It is worth noting that the pure quantum contribution to the total occupation of the noncondensate remains finite and directly measurable by particle detectors at $T \to 0$. It is well-known as the quantum depletion of the condensate [42,63] and possesses a nontrivial statistics of fluctuations [34]. Such fluctuations in the total occupation of the noncondensate have been already directly observed and sampled [48]. The pure quantum contribution to the covariance matrix given by Eqs. (41) and (40) describes, via the characteristic function (23) and the probability distribution (27), even more intriguing statistics of joint fluctuations in the excited-state occupations of different groups of excited states. It also can be directly accessed in the experiments on atomic boson sampling. Note that the above statistics is easy to compute in the preferable basis of the eigen-squeeze states defined in Eqs. (38) since the covariance matrix $\bar{G}_Q$ in Eq. (41) corresponds to completely independent fluctuations of M atomic states with single-mode squeezing. However, that statistics observed in an arbitrary set of bare-particle excited states becomes ♯P-hard for computing due to an interference caused by the unitary transformation between eigen-squeezed and bare-particle states. As follows from Eqs. (41) and (42), the pure quantum and complimentary thermal contributions both explicitly involve the irreducible squeezing matrix Λ_r. Thus, a simultaneous appearance (in the bare-particle states) of the squeezing (due to interaction) and the interference (due to unitary mixing of the eigen-squeezed states) is responsible for the ♯P-hardness of computing the atomic boson sampling statistics.

It is known that in the absence of squeezing, a unitary mixing of modes fed with thermal light does not make boson sampling ♯P-hard. Apparently, the presence of only asymptotically small squeezing in all eigen-squeezed modes, $r_j \ll 1$, would not help either. The system has to provide significant, not necessarily of order of unity ($\tanh r_j \sim 1$), but still large enough squeezing in some fraction, M', out of all M eigen-squeezed modes. The latter implies that the asymptotic parameter responsible for the ♯P-hardness of computing atomic boson sampling is limited by a dimension of a subspace in the Hilbert space of excited states associated with an intersection of the subspace, comprised by M' significantly squeezed eigen-squeezed states, and the subspace of states constituting significantly occupied quasiparticles. Indeed, only those two sets of eigenmodes, associated with the eigenvectors of the Hamiltonian and the eigenvectors of the squeezing matrix, constitute and provide the unique, unambiguous reference frame and characterization of the system.

Please note that the dominant effect of the many-body interaction and interference on the quantum statistics of the atomic boson sampling in Eqs. (23), and (27) is accurately described by the above Bogoliubov-Popov approach only within the first-order approximation over the weak interaction parameter $\sqrt{a^3 N/V} \ll 1$ and far from the critical region, i.e., at such a low temperature T that $(T_c - T)/T_c \gg a(N/V)^{1/3}$. In fact, the last inequality also sets the range of validity of the mean-field approximation where, according to the Ginzburg-Levanyuk criterion [109,110], a mean value of the order parameter of the BEC phase transition is larger than its fluctuations. The only approximations we adopted in the present paper for the analysis of the atomic boson sampling statistics are the ones needed for validity of the Bogoliubov model. (We do not elaborate on them here since they had been analyzed in detail and scrutinized in many works and reviews; see, for instance, Refs. [42,43,82] and references therein.) Small higher-order corrections due to the main s-wave interaction and other factors (such as the presence of other minor interactions, a drift and fluctuations of the trapping potential, external magnetic field, temperature, sampled modes and other setup parameters, losses of atoms, and other nonequilibrium processes) as well as a detector inaccuracy and other imperfections require an additional, separate analysis. Those imperfections are always present in real experimental systems, including a usual optical interferometer, and can wash out the ♯P-hardness if they are too large. Their analysis in the case of the photonic boson sampling has been addressed in a number of papers. A similar analysis in the case of the atomic boson sampling in a BEC trap is not available yet, but needs to be done later on.

The important point is that the ♯P-hardness of computing the atomic boson sampling statistics due to appearance of the Hafnian is not just a feature of the Bogoliubov approximation. The characteristic function similar to the one within the Bogoliubov approximation, Eq. (23), also arises in the exact nonperturbative theory of critical fluctuations which is based on the nonpolynomial diagram technique [45–47] (see, for instance, Eq. (54) in Ref. [47]). In virtue of the Hafnian master theorem (28) (see Appendix B), it describes the same ♯P-hardness of computing the joint occupation distribution—the one originating from ♯P-hardness of the Hafnian of a matrix associated with an appropriate covariance matrix.

Compared to the exact general analysis [45–47] (which consistently includes the effects of critical fluctuations in the critical region of phase transition on the many-body statistics), the Bogoliubov approximation (which is a mean-field theory of the first-order with respect to the interaction parameter) neglects by critical fluctuations and multipartite higher-order correlations, but provides a simplified covariance matrix G accounting only for fluctuations via independent quasiparticles. Thus, the difference between the approximate and exact theories is that the Bogoliubov approximation gives an explicit expression for the covariance matrix G and, hence, for the characteristic function, while within the exact general analysis calculating the covariance matrix G in an explicit form is difficult. The detailed theory (within the Bogoliubov approximation), that provides analytical calculation of the joint probability distribution of excited state occupations presented above, constitutes the subject of the paper. A nonperturbative theory of critical fluctuations is much more involved and is beyond the scope of the present paper.

What is really surprising is that, despite tremendous simplifications due to the aforementioned rough omissions, the atomic boson sampling statistics within the Bogoliubov approximation (hence, very far from the critical point of the BEC phase transition) remains within the same top-level ♯P-hard computational complexity class as within the exact analysis (near the critical point). In other words, one may think that tremendous complications in the many-body quantum theory of critical phenomena in phase transitions due to the nonperturbative multipartite-correlation nature of anomalous critical fluctuations could be responsible for placing the many-body quantum statistics into the top-level complexity class. Yet the latter is not the case. The interaction via Bogoliubov coupling and interference of bare-particle excited states within the scope of the quasiparticle approach are enough for raising the atomic boson sampling statistics to the top-level, ♯P-hard complexity class.

Different manifestations of ♯P-hardness of atomic boson sampling, such as various interference and correlation properties of joint moments and cumulants or scaling associated with the Hafnian of finite-size correlation matrices, can be tested experimentally. They should be compared against some classical computer simulations based on classical algorithms, approximations, or mockups ranging from oversimplified or already known ones to more and more sophisticated ones. Those classical aspects of simulations as well as the design of particular BEC experiments and atom number detectors are beyond the scope of the present paper. Here we focus on the understanding and analytical theory of the actual quantum statistical physics of this many-body system and, except fragmentary comments, leave all experimental, technological, engineering, applied, and verification aspects of this multiside problem for future papers and other researchers.

It is worth noting that in the real experiments on the atomic boson sampling, the interaction parameter should not be tuned to zero but should be kept finite to provide (i) a common condensate extending over the entire BEC trap and (ii) significant Bogoliubov couplings (6) over a large enough set of atomic states. Those two conditions favor spreading the nontrivial correlations and multimode squeezing over a large number of bare excited atomic states and, hence, achieving a large size of the correlation and squeezing matrices specifying the matrix under the Hafnian. In principle, one should try to make that number or size as large as possible since the ♯P-hardness of computing the atomic boson sampling implies an exponential (as opposed to polynomial) time of computing with respect to that asymptotic parameter.

Obviously, in the limit of an exponentially small interaction parameter the Bogoliubov couplings in Eq. (6) and squeezing in Eq. (18) vanish. So, the aforementioned ♯P-hard complexity vanishes in an ideal Bose gas within the grand canonical ensemble approximation. In the canonical ensemble, some nontrivial correlations between equilibrium occupations of the excited particle states of the trap exist even in the ideal gas due to the total particle number constraint, $N = \text{const}$. They are related to the known critical fluctuations in the total noncondensate or condensate occupation in the ideal gas confined in a mesoscopic trap [44,111].

The ♯P-hardness also disappears in some exactly soluble cases or when the matrix C in Eq. (27) is degenerate so the Bogoliubov coupling matrix (6) has a special or degenerate form such that the associated Hafnians or permanents, defining the joint probability distribution in accord with the Hafnian or permanent master theorems, (28) or (30), are computable in polynomial time (e.g., via fully polynomial randomized approximation scheme [39] or recursively, like permanents in Ref. [112]).

VII. TESTING BOSON SAMPLING IN THE ATOMIC BEC TRAP AND COMPARING IT WITH PHOTONIC-INTERFEROMETER EXPERIMENTS

The present paper is devoted to an investigation of the computational complexity of calculating the joint probability distribution of excited state occupations in the interacting BEC gas and the related atomic boson sampling. The atomic BEC trap can be viewed as a boson-sampling platform alternative to a photonic interferometer. In both systems, the output multivariate statistics is associated with the ♯P-hard for computing Hafnians of complex-valued, easily controllable matrices. The latter allows one to vary the output statistics over a wide range. It is remarkable that computing the atomic boson sampling in an interacting equilibrium many-body system turns out to be similar to computing the Gaussian boson sampling of noninteracting photons in a linear interferometer. That is why we discuss its relation to the known photonic Gaussian boson sampling in a linear interferometer.

We emphasize that the system of interacting atoms in the BEC trap does not need (a) any external source of input bosons in any quantum (Fock, squeezed, etc.) states, (b) control of system parameters and gates, or (c) any other type of processing usually associated with quantum computers or simulators. In principle, after each measurement of the occupations of the excited state or coarse-grained groups of them, for instance, via a simultaneous optical multidetector imaging, the system of interacting atoms returns back to the equilibrium state (that is, resets itself, if the atoms were not removed from the trap, or is reloaded into the trap, if the atoms were released from the trap for occupations measurement) and becomes ready for the next multi-detector measurement of the joint atomic occupations. In other words, this is not a quantum computer or simulator of some input signal or some artificial, controlled process. The combined system of atoms in the BEC trap and detectors works as a random string generator, namely, it generates random strings of the excited state occupation numbers obeying the joint probability distribution (27) given by the ♯P-hard for computing Hafnian $\mathrm{haf}\tilde{C}(\{n_k\})$. One just need to perform accurate multidetector measurements, while the system of atoms in the BEC trap processes its own persistent equilibrium fluctuations and does not require any fine tuning or adjustment of various input, coupling, processing, or interaction parameters. This is not the case for the usually discussed nonequilibrium quantum simulators or processors, including setups based on Gaussian boson sampling in a linear interferometer, which require sophisticated on-demand sources of photons in squeezed states, lossless propagation through numerous beam splitters, couplers, phase shifters, etc.

In other words, the excited atoms naturally fluctuate and are squeezed inside the trap even in a thermal state. This allows one to eliminate the nonequilibrium state or dynamics and sophisticated external sources of squeezed or single bosons (required for photonic sampling) from the atomic sampling experiments. So, the losses of bosons on the input-output propagation, which constitute the main limitation factor in photonic sampling, are no more an issue for atomic sampling. It remains just to measure the distribution of atoms over the excited state subset by means of appropriate detectors.

In fact, an absence of the synchronized, on-demand single-photon sources for feeding the input channels of the interferometer is the reason for a recent shift from an original proposal [1,2] to a Gaussian boson sampling scheme that utilizes a squeezed (or more general, Gaussian) photon input provided by already available on-demand sources based on a parametric down-conversion [9,10,31]. For the BEC-trap platform, such a squeezed input is provided by nature itself due to the Bogoliubov coupling even in the box trap as has been shown in Ref. [33]. So, the BEC-trap platform is closer to and should be compared with the Gaussian boson sampling.

It would be very interesting to study experimentally various phenomena associated with atomic boson sampling by simultaneously measuring the occupations of the excited states or coarse-grained groups of them, say, via a multidetector imaging based on the light transmission through or scattering from the atomic cloud. The transmission imaging is based on the absorption or dispersion caused by atoms [48,58,81,113,114]. A scattering or fluorescence imaging [115], including a Raman one, could be facilitated by exciting modes, mimicking excited states, via lasers and cavities. Such experiments could be devised similar to optical imaging of the local atom-number fluctuations [57,58,73,74,114–117].

Detecting a particle number in each excited state or group of states can be facilitated by raising the total number N of particles loaded into the trap since the excited-state occupations scale as $(N - \langle N_0\rangle)/M$. Raising $N - \langle N_0\rangle$, say, from 10^2 to 10^4 multiplies the occupations by 100. The asymptotic parameter of complexity depends on the number of excited states or groups of states involved in the squeezing (due to interaction) and interference (due to mixing) as well as on the number of the excited atomic states or their groups to be measured by detectors, M, which is similar to the number of channels in the interferometer. That parameter is neither the total number of atoms in the trap N nor the number of bosons (noncondensed atoms) in the system $N - \langle N_0\rangle$.

Measuring with a single atom resolution is challenging, but a nearly single atom resolution had been achieved [115–118], though it is not required for showing quantum advantage since boson sampling is ♯P-hard for computing even if it is done with threshold detectors. Such detectors provide just two measurement outcomes—either zero or nonzero occupation in a given mode. The threshold boson sampling is described by torontonians (their computing is not easier than computing the Hafnians) and still possesses a quantum advantage [11,22,32].

Technically, such experiments could be devised similar to recent experiments on the optical imaging of the local atom-number fluctuations in BEC gases [57,58,73,74,114,115]. An optical imaging with a multidetector recording could give information on the joint simultaneous occupations of different cells or modes of the trap. Of course, particles in the condensate ψ_0, which is orthogonal to the excited states ψ_k, should not be countered. The cells or modes could represent groups of the excited states selected and composed from any basis in the single-particle Hilbert space. Importantly, the result for their joint occupation probability distribution in Eqs. (23)–(29) and (33) is universal relative to a choice of such a basis. A basis change amounts to just an additional unitary rotation, i.e., to an appropriate choice of the symplectic Bogoliubov matrix R, Eq. (1).

Importantly, various coarse-grained measurements are also fully appropriate. In other words, the experiments could be aimed at boson sampling of occupations of any-basis excited states, not necessarily, say, single-particle states of an empty trap, and even any subset of states (irrespective to the other states) or a set of groups (bunches) of states, that is, not necessarily all states or each state, respectively, of, for instance, the lower miniband formed by the qubit-well states discussed in Sec. II. Such incomplete experiments on a marginal or coarse-grained, respectively, particle-number distribution constitute a set of realistic tests on manifestations of ♯P-hardness of computing joint occupations statistics of excited states. A related incomplete statistics is given by the same general formula for the characteristic functions (23) and (28) due to its universality as is explained in the end of Sec. IV.

Remarkably, separation of the noncondensate from the condensate, counting the total number of atoms in the excited states (noncondensate) and accumulating its statistics has been demonstrated experimentally [48]. The only additional step, required for the atomic boson sampling experiments, is to split the noncondensed atoms into some smaller groups and measure atom numbers in the preselected states or groups of states. That splitting could be based, for example, on splitting the entire volume of the trap into a set of spatial cells (as discussed for the multiqubit trap in Sec. II, Fig. 1) or on splitting atoms into the groups with different subsets of velocities (cells in the momentum space). In both cases, the atom-number measurement could be done with some kind of multidetector imaging. For instance, one could switch off the confining trap and let the cloud of atoms expand freely, similar to the usual time-of-flight experimental technique. Then, one just needs to take a sequence of multidetector images in short intervals of time and fitly interpret them via the expansion kinetics. Such a technique would allow one to distinguish different spatial and/or momentum groups of atoms and measure their occupations. However, neither an experimental demonstration of the suggested atomic boson sampling nor a design of a setup and atom number detectors for such an experiment is the subject of the present paper.

VIII. CONCLUSIONS

(i) We find the characteristic function (23) for the fluctuations of the excited-particle-state occupations. It is the universal determinantal function of the normally ordered covariance matrix (24). The function (23) is easy to compute in polynomial time by means of Gaussian elimination for any given values of its variables $\{z_k\}$. We calculate the covariance matrix (24) and present its irreducible form, Eqs. (40)–(42), via the eigenvalues and eigenvectors of the squeezing matrix given in Eqs. (17).

(ii) We formulate the Hafnian master theorem (28), which is a Hafnian's analog and generalization of the classical MacMahon master theorem on matrix permanents.

(iii) Computing a Fourier transform of the characteristic function (23), that is, the corresponding joint probability distribution (27) for any given values of the occupation numbers $\{n_k\}$, amounts to computing the matrix Hafnians as per Eq. (28) (see Appendix B) and is ♯P-hard. Despite a paradigm stating that a function and its Fourier transform contain the same information, it is clear that this ♯P-hardness appears due to multiple Fourier integration (cf. a permanent's integral representation [40]). The point is that the information encrypted in the probability of occurrence of just one set of the occupation numbers $\{n_k\}$ corresponds to the information encrypted in the values of the characteristic function at an exponentially large (with respect to $n = \sum_k n_k$) number of points, that is, an exponentially large subset of points in the space of Fourier variables $\{z_k\}$.

(iv) Conceptually, the particle sampling in the excited states of a BEC trap and the Gaussian photon sampling in an interferometer are on the same footing. However, due to the presence of the interparticle interaction and the condensate in the BEC gas, the Bogoliubov coupling (6) results in a self-induced multimode squeezing in the many-body system of noncondensed atoms. It is described by the Bogoliubov transformation (14)–(18) that, in general, includes not only the diagonal squeezing parameters $r_{k,k}$ corresponding to the intramode squeezing but also all of the off-diagonal squeezing parameters $r_{k,k'}$ corresponding to the intermode squeezing between any two excited atomic modes k and k'.

(v) There is a remarkable difference between the atomic and photonic boson samplings: Due to many-body fluctuations and interparticle interaction, the atomic sampling in the BEC trap is associated with the ♯P-hard Hafnians even for a thermal, equilibrium state (without any particle source) while a nonthermal source of squeezed or Fock photons is required to get ♯P-hard Hafnians in the linear interferometer.

(vi) It is worth employing the characteristic function and cumulant analysis, which constitutes a well-known comprehensive tool in statistics [90–93] and is sketched above for the boson sampling in Eqs. (26)–(36), for (a) ruling out mockups, such as with nonsqueezed states or distinguishable bosons, (b) verifying that incoherent processes, boson loss, technical noise, detector dark counts, or other imperfections do not wash out the ♯P-hardness of sampling. The tools currently in use are based on the Bayesian test for a subsystem of modes [31,103], lower-order marginal distributions, truncation of high-order correlations and polynomial approximations [31,32,104–106], quasiprobability distributions, grouped correlations and phase-space methods [29,107], generalized bunching [14,15], etc.

(vii) The results in Eqs. (23)–(27) show that boson-sampling experiments could be based on any general-case BEC trap, for example, the multiqubit BEC trap formed by a finite number of single-qubit cells (Fig. 1).

After a recent successful experiment [48] on measuring fluctuations in the total occupation of the noncondensate, it remains just to split the noncondensate into a few separate fractions and measure, via some multidetector imaging technique, the joint fluctuations in the atom numbers of these fractions. Such experiments promise discovery of new quantum many-body effects which are manifestations of the computational ♯P-hard complexity of quantum many-body statistics and are beyond simple particle analogs of the effects like a Hong-Ou-Mandel one. They are doable at the present stage of the magneto-optical trapping and detection technology and would be valuable for understanding fundamental properties of the interacting many-body quantum systems directly relevant to quantum advantage. The ultimate experiments with an increasingly large number of the noncondensate fractions are very challenging. Of course, at the current, initial phase of this field of research, it remains unknown exactly how to achieve the quantum advantage using the BEC experiments. The main open problem is a development of a multidetector imaging technique for simultaneous measurement of excited-state occupations.

Overall, the analysis above goes far beyond the existing photon sampling studies in a linear interferometer. It ushers researchers from different fields to initiate exploring and designing the ♯P-hard complexity in their own interacting systems of various particles and fields.

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APPENDIX A: CHARACTERISTIC FUNCTION OF THE JOINT PROBABILITY DISTRIBUTION OF THE EXCITED-STATE ATOM NUMBERS

Here we derive the characteristic function in Eq. (23):

$$\Theta(\{z_k\}) = \frac{1}{\sqrt{\det[\mathbb{1} - (Z-\mathbb{1})G]}}, \quad Z \equiv \bigoplus_{k=1}^{M} \begin{bmatrix} z_k & 0 \\ 0 & z_k \end{bmatrix},$$
$$G = RDR^\dagger + \frac{RR^\dagger - \mathbb{1}}{2}, \quad D = \bigoplus_{j=1}^{M} \frac{1}{e^{E_j/T}-1} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}. \tag{A1}$$

The diagonal matrix D is determined by the mean occupation numbers of the quasiparticle excitations with energies E_j. The $2M\times 2M$ matrix R describes the Bogoliubov transformation from the vector $V_{\hat{b}} \equiv (.., \hat{b}_j^\dagger, \hat{b}_j, ..)^T$ of the quasiparticle creation and annihilation operators to the vector $V_{\hat{a}} \equiv (.., \hat{a}_k^\dagger, \hat{a}_k, ..)^T$ of the particle creation and annihilation operators:

$$V_{\hat{a}} = R\, V_{\hat{b}}. \tag{A2}$$

First, we formulate the symplectic property of the matrix R: Since the Bogoliubov transformation preserves the canonical Bose commutation relations for the creation and annihilation operators, it obeys the following relation, involving the block-diagonal matrix Ω:

$$R\,\Omega\,R^T = \Omega, \quad \Omega \equiv \bigoplus_{j=1}^{M} \begin{bmatrix} 0 & +1 \\ -1 & 0 \end{bmatrix}. \tag{A3}$$

Taking into account that the Bogoliubov transformation (A2) simultaneously alters the pairs of Hermitian conjugated operators and, hence, satisfies the relation

$$R^T = AR^\dagger A, \quad A \equiv \bigoplus_{j=1}^{M} \sigma_x, \quad \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \tag{A4}$$

the symplectic property may also be rewritten as follows:

$$R\left(\bigoplus_{j=1}^{M} \begin{bmatrix} +1 & 0 \\ 0 & -1 \end{bmatrix}\right) R^\dagger = \bigoplus_{j=1}^{M} \begin{bmatrix} +1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{A5}$$

Next, we prove that the matrix $G = (G_K^{K'})$ in Eqs. (A1) is the covariance matrix defined as the statistical average of the normally ordered product of two particle creation or annihilation operators:

$$\left(G_{r,k}^{r',k'}\right) = (\langle{:}\hat{a}_{r,k}^\dagger\, \hat{a}_{r',k'}{:}\rangle) = \begin{bmatrix} \ddots & \vdots & \vdots & \\ \cdots & \langle \hat{a}_k^\dagger \hat{a}_{k'}\rangle & \langle \hat{a}_k^\dagger \hat{a}_{k'}^\dagger\rangle & \cdots \\ \cdots & \langle \hat{a}_k \hat{a}_{k'}\rangle & \langle \hat{a}_{k'}^\dagger \hat{a}_k\rangle & \cdots \\ & \vdots & \vdots & \ddots \end{bmatrix}. \tag{A6}$$

Its entries $G_K^{K'}$ are enumerated by the double indices $K = (r,k)$ for rows and $K' = (r',k')$ for columns. A Nambu-type index r (or r') acquires two values: 1, 2. For any operator $\hat{\mathcal{O}}$, it denotes that the same operator, $\hat{\mathcal{O}}_r = \hat{\mathcal{O}}$, if $r=1$ or its Hermitian conjugate, $\hat{\mathcal{O}}_r = \hat{\mathcal{O}}^\dagger$, if $r=2$. It is related to the (2×2)-block structure of the matrix. We assume $\langle \hat{a}_k\rangle = 0$. The diagonal matrix $Z = \mathrm{diag}(\{z_K\})$ consists of the pairs of the same variable $z_{r,k} = z_k = e^{iu_k}$ along the diagonal.

We mostly consider the system of a finite number, M, of the excited particle modes. So, the A, D, R, G, Ω, and Z are essentially the $2M\times 2M$ matrices. Yet, the method below can be easily extended to the case of an arbitrary countable set of an infinite number of excited modes.

Calculation of the characteristic function (for details of its definition and properties, see Refs. [90–93] and references therein) is similar to the calculation described in Ref. [34] and is based on the Wigner transform technique [99–101]. The Wigner transformation casts an operator-valued function $F(\hat{a}^\dagger, \hat{a})$ of the creation and annihilation operators $\hat{a}^\dagger$ and $\hat{a}$ into a complex-valued function W_F of the associated variables α^* and α as follows:

$$W_F(\alpha^*, \alpha) = \int_{\mathbb{C}} e^{-\gamma\alpha^* + \gamma^*\alpha}\, \mathrm{Tr}[e^{\gamma\hat{a}^\dagger - \gamma^*\hat{a}} F(\hat{a}^\dagger, \hat{a})] \frac{d^2\gamma}{\pi}. \tag{A7}$$

It allows one to represent the trace of an operator product $\hat{F}\hat{G}$ via a complex integral, $\mathrm{Tr}\,(\hat{F}\,\hat{G}) = \pi^{-1}\int W_F\, W_G\; d^2\alpha$. The above formulas are written in the single-mode case. In the multimode case, they include the multiple integrals. In particular, the characteristic function, $\Theta(\{u_k\}) \equiv \mathrm{Tr}(e^{i\sum_k u_k \hat{n}_k}\hat{\rho})$, has the following Wigner representation:

$$\Theta\big(\{u_k\}\big) = \int_{\mathbb{C}^M} W_{\{n_k\}}(\{\alpha_k^*, \alpha_k\}) W_\rho(\{\alpha_k^*, \alpha_k\}) \prod_{k=1}^{M} \frac{d^2\alpha_k}{\pi}. \tag{A8}$$

It is easy to calculate the Wigner transform of the statistical operator $\hat{\rho} = e^{-\sum_j E_j \hat{b}_j^\dagger \hat{b}_j/T}/\mathrm{Tr}\{e^{-\sum_j E_j \hat{b}_j^\dagger \hat{b}_j/T}\}$ as follows:

$$W_\rho\big(\{\beta_j^*, \beta_j\}\big) = \prod_{j=1}^{M}\left(2\tanh\frac{E_j}{2T}\right) \exp\left[-2\beta_j^*\beta_j \tanh\frac{E_j}{2T}\right]$$
$$= e^{-V_\beta^T B V_\beta} \prod_{j=1}^{M}\left(2\tanh\frac{E_j}{2T}\right);$$
$$V_\beta \equiv (\ldots, \beta_j^*, \beta_j, \ldots)^T, \quad B = \bigoplus_{j=1}^{M} \sigma_x \tanh\frac{E_j}{2T}. \tag{A9}$$

Here the complex variables β_j^* and β_j are associated with the quasiparticle operators $\hat{b}_j^\dagger$ and $\hat{b}_j$, respectively, and constitute vector V_β of size $2M$, which is the counterpart of vector $V_{\hat{b}}$ introduced in Eq. (A2) above.

The Wigner transform of the operator $\exp(i\sum_k u_k \hat{a}_k^\dagger \hat{a}_k)$, whose average equals the characteristic function, is

$$W_{\{n_k\}}(\{\alpha_k^*, \alpha_k\}) = \prod_{k=1}^{M} \frac{2}{z_k+1} \exp\left(2\alpha_k^*\alpha_k \frac{z_k-1}{z_k+1}\right)$$
$$= \exp\left(V_\alpha^T \frac{Z-\mathbb{1}}{Z+\mathbb{1}} A V_\alpha\right) \prod_{k=1}^{M} \frac{2}{z_k+1};$$
$$V_\alpha \equiv (\dots, \alpha_k^*, \alpha_k, \dots)^T,$$
$$\frac{Z-\mathbb{1}}{Z+\mathbb{1}} = \bigoplus_{k=1}^{M} \frac{z_k-1}{z_k+1}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}$$
$$= \bigoplus_{k=1}^{M} \frac{e^{iu_k}-1}{e^{iu_k}+1}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}. \quad \text{(A10)}$$

Similar to Eqs. (A9), the complex variables α_k^* and α_k are associated with the particle operators $\hat{a}_k^\dagger$ and $\hat{a}_k$, respectively, and constitute vector V_α of size $2M$, which is the counterpart of the vector $V_{\hat{a}}$ introduced in Eq. (A2) above. Each argument of the characteristic function $u_k, k = 1, \dots, M$, appears, in the form of the exponential variable $z_k = e^{iu_k}$, twice in the entries of the kth (2×2)-block of the block-diagonal $2M\times2M$ matrix $(Z-\mathbb{1})(Z+\mathbb{1})^{-1}$.

Now we employ the property of the Wigner transform highlighted in Ref. [101]: The linear similarity transformation of the operator functions carries over to their Wigner functions. It allows us to find the Wigner transform $W_\rho(\{\alpha_k^*, \alpha_k\})$ for Eq. (A8) by substituting variables $V_\beta = R^{-1}V_\alpha$ into Eqs. (A9). As a result, Eq. (A8) takes the following explicit form:

$$\Theta(\{z_k\}) = \int_{\mathbb{C}^M} \exp\left[-V_\alpha^T(\tilde{B} - \frac{Z-\mathbb{1}}{Z+\mathbb{1}}A)V_\alpha\right]$$
$$\times \prod_{k=1}^{M} \frac{4\tanh(E_k/2T)}{z_k+1}\frac{d^2\alpha_k}{\pi},$$
$$\tilde{B} \equiv (R^T)^{-1}BR^{-1}. \quad \text{(A11)}$$

The matrix $\tilde{B}$ is matrix B written in the particle basis as opposed to the quasiparticle basis.

Changing the integration variables to $\mathrm{Re}\,\alpha_k$ and $\mathrm{Im}\,\alpha_k$ and applying a well-known formula for the Gaussian integral $\int_{\mathbb{R}^n} \exp(-\mathbf{x}^T S\mathbf{x}) \prod_{j=1}^n dx_j = \pi^{n/2}/\sqrt{\det S}$ with a symmetric matrix $S = S^T$ whose real part $\mathrm{Re}\,S$ is positively definite, we get

$$\Theta = \frac{2^M \prod_{j=1}^M \tanh\frac{E_j}{2T}}{\sqrt{(-1)^M \det\left(\tilde{B} - \frac{Z-\mathbb{1}}{Z+\mathbb{1}}A\right)\prod_{k=1}^M (z_k+1)^2}}$$
$$= \frac{2^M}{\sqrt{(\det\tilde{B})^{-1}\det\left(\tilde{B} - \frac{Z-\mathbb{1}}{Z+\mathbb{1}}A\right)\det(Z+\mathbb{1})}}. \quad \text{(A12)}$$

The last equality follows from representing the left-hand-side products as the determinants of the appropriate matrices:

$$\prod_{j=1}^{M} \tanh^2(E_j/2T) = (-1)^M \det B = (-1)^M \det\tilde{B},$$
$$\prod_{k=1}^{M} (z_k+1)^2 = \det(Z+\mathbb{1}). \quad \text{(A13)}$$

The matrices B and $\tilde{B}$ have equal determinants, $\det B = \det\tilde{B}$, since the Bogoliubov transformation preserves the commutation relations and, hence, its matrix R is simplectic, which implies $\det R = \det R^T = 1$. Multiplying the matrices in the denominator, we get

$$\Theta(\{z_k\}) = \frac{1}{\sqrt{\det\left(\frac{\tilde{B}^{-1}A+\mathbb{1}}{2} - Z\frac{\tilde{B}^{-1}A-\mathbb{1}}{2}\right)}}$$
$$= \frac{1}{\sqrt{\det\left(\mathbb{1} - (Z-\mathbb{1})\frac{RB^{-1}R^TA-\mathbb{1}}{2}\right)}}. \quad \text{(A14)}$$

The inverse of the block-diagonal matrix B is straightforward to calculate as $B^{-1} = A(1+2D)$. As a result, in virtue of Eq. (A5), Eq. (A14) acquires the form of Eq. (A1). This completes the proof of the first part of Eqs. (A1).

The formula for the characteristic function (A1) is derived above for the case of a finite number of excited states M. However, the final result does not explicitly depend on the dimension M of the Hilbert space on which the bosons live. So, the formula in Eqs. (A1) can be also applied to a Bose system with an infinite number of the excited states. Of course, the finite-size matrix definitions and the finite products employed above should be modified accordingly to fit the case of an infinite countable dimension.

Derivation of the formula for the normally ordered covariance matrix G [defined in Eqs. (A6)], that is, the second part of Eqs. (A1), is straightforward. Consider unordered covariance matrices $\tilde{G}$ of particle and quasiparticle operators which are defined as follows:

$$\tilde{G}_{\hat{a}} \equiv \langle V_{\hat{a}}\, V_{\hat{a}}^\dagger\rangle = \begin{bmatrix} \ddots & \vdots & \vdots & \\ \cdots & \langle\hat{a}_k^\dagger\hat{a}_{k'}\rangle & \langle\hat{a}_k^\dagger\hat{a}_{k'}^\dagger\rangle & \cdots \\ \cdots & \langle\hat{a}_k\hat{a}_{k'}\rangle & \langle\hat{a}_k\hat{a}_{k'}^\dagger\rangle & \cdots \\ & \vdots & \vdots & \ddots \end{bmatrix},$$
$$\tilde{G}_{\hat{b}} \equiv \langle V_{\hat{b}}\, V_{\hat{b}}^\dagger\rangle = \begin{bmatrix} \ddots & \vdots & \vdots & \\ \cdots & \langle\hat{b}_j^\dagger\hat{b}_{j'}\rangle & \langle\hat{b}_j^\dagger\hat{b}_{j'}^\dagger\rangle & \cdots \\ \cdots & \langle\hat{b}_j\hat{b}_{j'}\rangle & \langle\hat{b}_j\hat{b}_{j'}^\dagger\rangle & \cdots \\ & \vdots & \vdots & \ddots \end{bmatrix}. \quad \text{(A15)}$$

They Bogoliubov transformation establishes the following relation between them:

$$\tilde{G}_{\hat{a}} = R\,\tilde{G}_{\hat{b}}R^\dagger. \quad \text{(A16)}$$

The normally ordered covariance matrix differs from the unordered one by a matrix representing the Bose commutator which has only one unity entry in each 2×2 block:

$$((\langle :\hat{a}^\dagger_{r,k}\hat{a}_{r',k'}:\rangle) = \tilde{G}_{\hat{a}} - \bigoplus_{j=1}^{M}\begin{bmatrix}0 & 0\\ 0 & 1\end{bmatrix},$$

$$((\langle :\hat{b}^\dagger_{r,k}\hat{b}_{r',k'}:\rangle) = \tilde{G}_{\hat{b}} - \bigoplus_{j=1}^{M}\begin{bmatrix}0 & 0\\ 0 & 1\end{bmatrix}. \tag{A17}$$

The quasiparticles are the independent, noninteracting boson excitations. The average occupation of their energy levels $\{E_j\}$ in the thermal, equilibrium state, $\hat{\rho} \sim \exp(-\sum_j E_j \hat{b}^\dagger_j \hat{b}_j/T)$, is given by the Bose-Einstein distribution $\langle \hat{b}^\dagger_j \hat{b}_j\rangle = (e^{E_j/T}-1)^{-1}$. So, the covariance matrix of the quasiparticle operators is exactly matrix D defined in Eq. (25), $D = (\langle :\hat{b}^\dagger_{r,k}\hat{b}_{r',k'}:\rangle)$.

Equations (A16) and (A17) immediately lead to the explicit formula for the normally ordered covariance matrix:

$$((\langle :\hat{a}^\dagger_{r,k}\hat{a}_{r',k'}:\rangle) = RDR^\dagger + R\left(\bigoplus_{j=1}^{M}\begin{bmatrix}0 & 0\\ 0 & 1\end{bmatrix}\right)R^\dagger - \bigoplus_{j=1}^{M}\begin{bmatrix}0 & 0\\ 0 & 1\end{bmatrix}. \tag{A18}$$

The last relation we need is

$$R\left(\bigoplus_{j=1}^{M}\begin{bmatrix}0 & 0\\ 0 & 1\end{bmatrix}\right)R^\dagger - \bigoplus_{j=1}^{M}\begin{bmatrix}0 & 0\\ 0 & 1\end{bmatrix} = R\left(\bigoplus_{j=1}^{M}\begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix}\right)R^\dagger - \bigoplus_{j=1}^{M}\begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix},$$

which is equivalent to the symplectic property of the Bogoliubov transform written in terms of matrices R and $R^\dagger$, Eq. (A5). It ensures that the last two terms in Eq. (A18) equal $(RR^\dagger - \mathbb{1})/2$, which yields the required result for the normally ordered covariance matrix:

$$((\langle :\hat{a}^\dagger_{r,k}\hat{a}_{r',k'}:\rangle) \equiv G = RDR^\dagger + \frac{RR^\dagger - \mathbb{1}}{2}. \tag{A19}$$

This completes the proof of the second part of Eqs. (A1).

The relation $R^\dagger = AR^TA$ linking transposed and Hermitian conjugated Bogoliubov transform matrices makes it obvious that the matrix AG is symmetric. Thus, the matrices $\tilde{C}(\{n_k\})$ appearing under the Hafnian in the occupation probabilities (27) and in the Hafnian master theorem (28) are all symmetric.

APPENDIX B: THE HAFNIAN MASTER THEOREM

Here we give a simple derivation of the Hafnian master theorem for an arbitrary covariance matrix G, Eqs. (A6):

$$\frac{1}{\sqrt{\det(\mathbb{1}+(\mathbb{1}-Z)G)}} = \sum_{\{n_k\}} \frac{\text{haf}\,(\tilde{C}(\{n_k\}))}{\sqrt{\det(\mathbb{1}+G)}}\prod_k \frac{z_k^{n_k}}{n_k!},$$

$$C = AG(\mathbb{1}+G)^{-1}. \tag{B1}$$

It establishes the Taylor series of the determinantal function $1/\sqrt{\det(\mathbb{1}+(\mathbb{1}-Z)G)}$ over its M variables $\{z_k|k=1,\dots,M\}$ at the point of origin $\{z_k=0\}$ and is the Hafnian's analog of the permanent master theorem of MacMahon [35]. Here the $(2n\times 2n)$-matrix $\tilde{C}(\{n_k\})$, $n=\sum_k n_k$, is built from matrix C via replacing the kth pair of rows with the n_k copies of the kth pair of rows for all $k=1,\dots,M$ and then replacing the k'th pair of columns in the $(n\times 2M)$ matrix, obtained at the first step, with the $n_{k'}$ copies of the k'th pair of columns for all $k'=1,\dots,M$.

The multiple Gaussian integrals have been intensively used in quantum field theory, many-body physics, and quantum optics for decades. An example is a neat analysis [108] of the intensity distribution among the vibronic bands in electronic spectra of polyatomic molecules, taking into account the rotation of the excited-state normal coordinates relative to those of the ground state (the Dushinsky effect). It involves the Gaussian integrals similar to the ones employed in the derivation of the Hafnian master theorem. In principle, the latter could be derived by an appropriate expansion of such integrals over the variables $\{z_k\}$. However, previous works did not target a generating function for the Hafnians and did not present the explicit general formula (B1), or (28), that expresses the Hafnian master theorem for an arbitrary symmetric matrix. It is worth noting also that a few first terms on the right-hand side of Eq. (B1) become elementary in the case of a small size of the $2n\times 2n$ matrix under the Hafnian in the coefficients of the Taylor expansion of the characteristic function since they can be represented via explicit polynomials of the G-matrix entries. The Hafnian master theorem in the explicit general form of Eqs. (B1), valid in the case of an arbitrarily large matrix size and aimed at the analysis of the ♯P-hardness of computing, has been missing until now. Yet, the large-size case and the formula (B1) are crucially important for the analysis of the ♯P-hardness of computing atomic boson sampling.

In fact, Eq. (B1) is an immediate consequence of the Wick's theorem, well-known in the quantum field theory [94,95]. One just needs to apply the Wick's theorem to the mixed partial derivatives of the characteristic function (A1):

$$\prod_k \frac{\partial^{n_k}}{\partial z_k^{n_k}} \frac{1}{\sqrt{\det(\mathbb{1}+(\mathbb{1}-Z)G)}}\Bigg|_{\{z_k=0\}} = \text{Tr}\left\{\hat{\rho}\prod_k\left[z_k^{\hat{n}_k-n_k}\prod_{j=0}^{n_k-1}(\hat{n}_k-j)\right]\right\}\Bigg|_{\{z_k=0\}};$$

$$\hat{\rho} = \frac{e^{-\hat{H}/T}}{\text{Tr}\{e^{-\hat{H}/T}\}}. \tag{B2}$$

If taken under the quantum-mechanical statistical average in the definition of the characteristic function $\Theta(\{z_k\}) = \text{Tr}\{\hat{\rho}\prod_k z_k^{\hat{n}_k}\}$, the mixed derivative can be written as above, via the products of n_k shifted occupation operators $\hat{n}_k - n_k + 1, \dots, \hat{n}_k = \hat{a}^\dagger_k\hat{a}_k$. For each mode k, in virtue of the Bose commutation relation $[\hat{a}_k, \hat{a}^\dagger_{k'}] = \delta_{k,k'}$, such a product is equal to the normally ordered product of the n_k annihilation operators and n_k creation operators, $\prod_{j=0}^{n_k-1}(\hat{n}_k - j) = (\hat{a}^\dagger_k)^{n_k}\hat{a}_k^{n_k}$. It suffices to find the trace in Eq. (B2) for equal variables $z_k = z = e^{iu} \to 0,\ k=1,\dots,M$. If the operator of the total number of excited particles $\hat{N} = \sum_k \hat{n}_k$ commuted with the Bogoliubov Hamiltonian $\hat{H}$, then we would get a usual average of a product of the creation or annihilation operators over a density matrix $\hat{\rho}_\mu \propto e^{-(\hat{H}-\mu\hat{N})/T}$ for a system with a related grand canonical Hamiltonian $\hat{H} - \mu\hat{N}$ and a chemical potential $\mu = iuT$. Since $\hat{N}$ and $\hat{H}$ do not commute, the average is a bit more involved but still can be easily calculated:

$$\prod_k \frac{\partial^{n_k}}{\partial z_k^{n_k}} \frac{1}{\sqrt{\det(\mathbb{1} + (\mathbb{1} - Z)G)}}\Bigg|_{\{z_k=0\}} = \frac{1}{\sqrt{\det(\mathbb{1} + G)}} \mathrm{Tr}\left\{ \frac{\hat{\rho} e^{\mu(\hat{N}-n)/T}}{\mathrm{Tr}\{\hat{\rho} e^{\mu(\hat{N}-n)/T}\}} \times \prod_k \left[(\hat{a}_k^\dagger)^{n_k} \hat{a}_k^{n_k}\right] \right\}\Bigg|_{z=0}. \quad \text{(B3)}$$

According to Wick's theorem, the average (the trace) in the right-hand side of Eq. (B3) is equal to the sum of all possible products of n two-operator contractions (averages)

$$\mathrm{Tr}\left\{ \frac{\hat{\rho} e^{\mu(\hat{N}-n)/T}}{\mathrm{Tr}\{\hat{\rho} e^{\mu(\hat{N}-n)/T}\}} :\hat{a}_{r,k}\hat{a}_{r',k'}: \right\}\Bigg|_{z=0} = C_{r,k}^{r',k'} \quad \text{(B4)}$$

of a given product of $2n$ creation or annihilation operators. As a result, and in virtue of the Hafnian's definition [37,96], originally given in the quantum field theory by Caianiello [97,98], we immediately get a concise final formula,

$$\mathrm{Tr}\left\{ \frac{\hat{\rho} e^{\mu(\hat{N}-n)/T}}{\mathrm{Tr}\{\hat{\rho} e^{\mu(\hat{N}-n)/T}\}} \prod_k \left[(\hat{a}_k^\dagger)^{n_k} \hat{a}_k^{n_k}\right] \right\}\Bigg|_{z=0} = \mathrm{haf}\,(\tilde{C}(\{n_k\})), \quad \text{(B5)}$$

in terms of the same Hafnian as the one in Eqs. (B1). Calculation of the two-operator average in Eq. (B4) via the Wigner transforms and Gaussian integrals is a straightforward exercise similar to the calculation of the characteristic function outlined in Appendix A. The result for the matrix $(C_{r,k}^{r',k'})$ in Eq. (B4) is $C = AG(\mathbb{1} + G)^{-1}$. It is precisely the matrix C employed in the theorem (B1).

The only additional, though obvious trick here is to represent the n_k pairs of the k-mode's creation or annihilation operators in Eq. (B3) via the n_k independent, completely degenerate (with exactly the same correlation properties) modes entering the matrix $\tilde{C}(\{n_k\})$ in Eq. (B1) as the n_k identical or degenerate pairs of the kth rows and the kth columns.

This completes the proof of the Hafnian master theorem, Eq. (B1). The latter immediately yields Eq. (27) for the joint probability distribution.

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