Grand-canonical condensate fluctuations in weakly interacting Bose-Einstein condensates of light

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Grand-canonical fluctuations of Bose-Einstein condensates of light are accessible to state-of-the-art experiments [J. Schmitt *et al.*, Phys. Rev. Lett. **112**, 030401 (2014).]. We phenomenologically describe these fluctuations by using the grand-canonical ensemble for a weakly interacting Bose gas at thermal equilibrium. For a two-dimensional harmonic trap, we use two models for which the canonical partition functions of the weakly interacting Bose gas are given by exact recurrence relations. We find that the grand-canonical condensate fluctuations for weakly interacting Bose gases vanish at zero temperature, thus behaving qualitatively similarly to an ideal gas in the canonical ensemble (or microcanonical ensemble) rather than the grand-canonical ensemble. For low but finite temperatures, the fluctuations remain considerably higher than for the canonical ensemble, as predicted by the ideal gas in the grand-canonical ensemble, thus clearly showing that we are not in a regime in which the ensembles are equivalent.

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I. INTRODUCTION

The experimental realization of Bose-Einstein condensates (BECs) of photons [1,2] opens new areas of research beyond Bose-Einstein condensates in ultracold atomic gases [3]: Theoretical investigations of photon condensates [4–8] are supplemented by research on quantum phase transitions of light [9], polariton condensates [10,11], and the observation of kinetic condensation in classical waves [12]. While in experimental realizations of BECs with ultracold atoms [13–15] the total number of atoms is (approximately) constant, for photon-BECs they vary enormously: The experiment of Ref. [16] shows grand-canonical statistics close to the ideal (noninteracting) gas.

Here we use the grand-canonical ensemble to describe such a BEC in the *presence of weak* interactions. Noninteracting bosons have been used to gain insights into number-theoretical questions [17,18] like the number partitioning problem, the question how many ways an integer can be expressed as sums of integers (for which deviations from Gaussian fluctuations have been investigated by applying methods developed for ultracold atoms to number theory both for bosons [19,20] and fermions [21]). A related question is how many possible ways there are to express a number as products of numbers [22]—here bosons in a logarithmic potential can be used [23,24].

For such number-theoretical problems, noninteracting particles are the obvious choice. However, for current experiments ideal Bose gases can only be an approximation. This would of course not be an issue if real gases always approached the ideal gas provided the interaction is weak enough. However, as we will see for low temperatures, even very weak interactions that hardly change the number or particles in the condensate can change the ideal-gas predictions for grand-canonical condensate fluctuations considerably.

Thus, the research on ideal Bose gases using the canonical ensemble or the microcanonical ensemble, for example, for fluctuations of ideal gases arguably is particularly useful if they survive weak interactions. Anomalous condensate fluctuations—condensate fluctuations that scale faster with particle number N than $N^{0.5}$ —are present in some (but not all) cases for ideal Bose gases: Only grand-canonical fluctuations become (for ultracold atoms unphysically) large for the three-dimensional trap investigated by Refs. [25–27], whereas the one-dimensional trap used by Ref. [28] does yield large fluctuations, even in the canonical ensemble. A systematic investigation for which dimensions and trap geometries anomalous fluctuations occur can be found for the canonical ensemble in Ref. [29] and for the microcanonical ensemble in Ref. [30].

When investigating interacting Bose gases [31–33], the question of whether anomalous fluctuations survive interactions has been an ongoing debate for quite some time. Weakly interacting Bose gases have been reported to show anomalous fluctuations if they are confined by a three-dimensional box potential [34], a system for which other authors have investigated the transition from anomalous to normal fluctuations [35]. Even for strongly interacting superfluids, anomalous fluctuations have been predicted [36] and explained on a fundamental level [37]. However, fundamental criticism of anomalous fluctuations has been described in Refs. [38,39]: In the thermodynamic limit anomalous fluctuations lead to diverging behavior of quantities important for stability considerations; the use of a second-order theory for calculating fourth-order quantities has also been criticized [38,39]. The divergences criticized in Refs. [38,39] only happen in the thermodynamic limit and they thus do not make statements on behavior for the finite particle numbers on which this paper (and many previous literature) focuses; here fluctuations can still be very large.

When deciding on an ensemble with which to describe a photonic BEC, the *grand-canonical ensemble* is the most obvious choice [16]. While for an ideal Bose gas there are differences between canonical (or microcanonical) and grand-

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canonical predictions for many thermodnamic quantities (cf. Refs. [40,41]), they are particularly large for fluctuations of the number of particles in the ground state (cf. Refs. [26,29,30]). The grand-canonical rms fluctuations Δn_0 of the ground state occupancy of an ideal Bose gas become unphysically large when one tries to describe atomic gases (at temperature T=0 they are larger than the total number of atoms, N). However, for photon BECs such high fluctuations can still be physical [16]. In this paper we investigate the influence of weak interactions on photon BECs when treated within the grand-canonical ensemble with two models that can be treated via exact recurrence relations on the level of the canonical ensemble (Refs. [42–44] and [35], respectively).

As such, the goal of the present paper is to look specifically at the influence of interactions on the grand-canonical fluctuations. In the grand-canonical description, it is assumed that the size of the reservoir is substantially larger than that of the subsystem. However, in photonic BECs, the size of the reservoir can be changed and made small, so the crossover from a grand-canonical ensemble towards a more canonical ensemble can be investigated. The study of this crossover falls outside the focus of the present paper, in which we want to isolate the effects of weak interactions from effects of reservoir size. Recent work [45] has suggested that weak interactions do affect the grand-canonical predictions in a manner similar to that observed experimentally in Ref. [16]. Rather than treating the interactions variationally as in Ref. [45], we will use model systems that allow us to take interactions into account in an exact way.

The paper is organized as follows: In Sec. II, we discuss interacting many-particle model systems for which the canonical partition functions are given by exact recurrence relations. We introduce the two models used in this paper in Sec. II C and Sec. II D. We present numerical and analytical results in Sec. III before the paper ends with the conclusions in Sec. IV.

II. CALCULATING THE GRAND-CANONICAL PARTITION FUNCTION USING EXACT RECURRENCE RELATIONS FOR THE CANONICAL PARTITION FUNCTIONS

A. Overview of Sec. II

We start this section with introducing the grand-canonical ensemble we use to calculate the thermodynamics of a photon BEC (Sec. IIB). As these equations are based on the *canonical* partition functions, we then discuss the two models we use to calculate the canonical partition functions via exact recurrence relations. The model introduced in Sec. IIC was previously used in Ref. [35], and the model of Sec. IID can be found in Ref. [44]. Both describe an interacting gas in a two-dimensional harmonic oscillator with N atoms at finite temperature T phenomenologically. When used to calculate grand-canonical partition functions, the model of Sec. II C converges for repulsive interactions, and the model of Sec. IID converges for attractive interactions. Both models are independent of each other, which helps to prevent making model-dependent statements. Both have the advantage of allowing us to treat a weakly interacting Bose gas in the grand-canonical ensemble using numerically exact recurrence

relations. For a very weakly interacting Bose gas with pairwise interactions, the model introduced in Sec. II C becomes exact for very low temperatures.

B. Grand-canonical ensemble: Partition function and fluctuations of the total number of bosons

We will first calculate the canonical partition functions for N particles $Z_N(\beta)$, where

$$\beta \equiv \frac{1}{k_B T},\tag{1}$$

and then proceed to calculate the grand-canonical partition function via

$$\Xi(\beta, z) = \sum_{n=0}^{\infty} z^n Z_n(\beta)$$

$$\simeq \sum_{n=0}^{N_{\text{max}}} z^n Z_n(\beta),$$
(2)

where we make sure that the sum has already converged at $n \approx N_{\rm max}$. As we will see later, this puts a constraint on the sign of the interaction we can model: One of our models can only treat attractive interactions, and the other only repulsive interactions.

The value for z is determined by asking the model to describe an experimental situation with an average number of particles of $N = \langle n \rangle$, where

$$\langle n \rangle = \frac{\sum_{n=0}^{N_{\text{max}}} n z^n Z_n(\beta)}{\sum_{n=0}^{N_{\text{max}}} z^n Z_n(\beta)}.$$
 (3)

Once z is determined (e.g., via bisection), the rms fluctuations of the total number of atoms,

$$\Delta N = \sqrt{\langle n^2 \rangle - \langle n \rangle^2},\tag{4}$$

also are accessible via

$$\langle n^2 \rangle = \frac{\sum_{n=0}^{N_{\text{max}}} n^2 z^n Z_n(\beta)}{\sum_{n=0}^{N_{\text{max}}} z^n Z_n(\beta)}.$$
 (5)

Here, and later, we use lowercase n to indicate the fluctuating total number of particles in the open subsystem in the grand-canonical ensemble. Capital N and ΔN denote the grand-canonical average and standard deviation of that number, respectively. When used in the context of the canonical ensemble, N denotes the fixed number of particles in that ensemble. Within the canonical ensemble, $\Delta N = 0$. The number of condensate atoms is noted as n_0 .

C. LTI model system

The low temperature interaction (LTI) model is based on Ref. [35].

For very weak interactions and very low temperatures we have

$$n_0 \simeq N,$$
 (6)

$$N_{\rm ex} \ll N,$$
 (7)

where

$$N_{\rm ex} \equiv N - n_0. \tag{8}$$

In this limit, we can treat the interaction between ultracold bosons in a harmonic trap analytically. Setting the single-particle ground-state energy to zero, the ground-state energy is proportional to the number of pairs $n_0(n_0 - 1)/2$ and the energy for one pair $2\alpha^1$

$$E_0(N) = \alpha N(N-1), \tag{9}$$

 $\alpha \ge 0.$

The fact that we are in a Bose-condensed state with a macroscopically occupied single-particle state is reflected in the energy scaling quadratically (rather than linearly) with particle number N. This scaling of the interaction energy can be found, for example, in the mean-field treatment of Bose-Einstein condensates via the Gross-Pitaevskii equation [56].

The total interaction energy is then approximately given by

$$E_{\text{int}}^{(1)}(n_0, N) = \alpha n_0(n_0 - 1). \tag{10}$$

Following Ref. [35], we also include the interaction between condensed atoms and noncondensed atoms

$$E_{\text{int}}^{(2)}(n_0, N) = \alpha n_0(n_0 - 1) + 2\alpha n_0 N_{\text{ex}}$$

= $\alpha (Nn_0 - n_0^2 - n_0)$. (11)

For the purpose of our grand-canonical calculations, we even can take a further step and treat interaction between excited atoms in the same way, yielding

$$E_{\text{int}}^{(3)}(n_0, N) = \alpha N(N - 1). \tag{12}$$

While Eq. (10) underestimates the total interaction energy, Eq. (12) overestimates it for finite temperatures. In the limit of extremely low temperatures all three energies coincide with the exact interaction energy if the interaction is pairwise as $n_0 = N$ at T = 0 for weak interactions:

$$E_{\text{int}}^{(j)}(n_0) = E_{\text{int}}^{\text{exact}}, \quad k_B T \ll \hbar \omega, \quad j \in \{1, 2, 3\}.$$
 (13)

For the excited atoms, that is, the noncondensed parts, we can then use the recurrence relation [57]

$$Z_N^{(\text{ex})}(\beta) = \frac{1}{N} \sum_{n=1}^N Z_1^{(\text{ex})}(n\beta) Z_{N-n}^{(\text{ex})}(\beta), \tag{14}$$

$$Z_0^{(\text{ex})}(\beta) \equiv 1; \tag{15}$$

for a two-dimensional (2D) harmonic oscillator we have

$$Z_1^{(ex)}(\beta) = \left(\frac{1}{1 - \exp(-\beta\hbar\omega)}\right)^2 - 1 \tag{16}$$

for the canonical partition functions. Derivations of the recurrence relation (14) can be found in Refs. [29,58–60].

The total canonical partition function is then given by

$$Z_{N}^{(j)}(\beta) = \sum_{n_{0}=0}^{N} \exp\left[-\beta E_{\text{int}}^{(j)}(n_{0}, N)\right] Z_{N-n_{0}}^{(\text{ex})}(\beta), \quad N \geqslant 1,$$
(17)

$$Z_0(\beta) \equiv 1. \tag{18}$$

The grand-canonical partition function then reads

$$\Xi^{(j)}(\beta, z) = \sum_{n=0}^{\infty} z^n Z_n^{(j)}(\beta).$$
 (19)

The canonical expectation for the average occupancy (k = 0) and higher moments (k > 1) are given by

$$\langle n_0^k \rangle_{N,j}^{\text{can}} = \frac{1}{Z_N^{(j)}(\beta)} \sum_{n_0=0}^N n_0^k \exp\left[-\beta E_{\text{int}}^{(j)}(n_0, N)\right] Z_{N-n_0}^{(\text{ex})}(\beta).$$
(20)

So far, this section has focused on the canonical ensemble with fixed total particle number N within the LTI model. In order to obtain the grand-canonical counterpart of Eq. (20), we have to add a grand-canonical average to obtain:

$$\langle n_0^k \rangle_j^{\text{gc}} = \frac{1}{\Xi^{(j)}(\beta)} \sum_{n=0}^{\infty} \langle n_0^k \rangle_{n,j}^{\text{can}} z^n Z_n^{(j)}(\beta). \tag{21}$$

While for attractive *atomic* BECs stability is an issue (see footnote 1), for a (so-far hypothetical) grand-canonical *photon* BEC with attractive pairwise interaction the grand-canonical partition function would diverge [see Eqs. (17) and (19)] because of contributions of arbitrarily high photon number, thus indicating the necessity to either rethink the modeling of such a system or restrict the experiments to a regime in which the grand-canonical ensemble is not valid.

D. BDL model system [42]

The model system of Brosens, Devreese, and Lemmens [42,61] (BDL) consists of *N* particles in a harmonic trap, with harmonic interactions between each pair of particles:

$$L(r_{j},\dot{r}_{j}) = \sum_{j=1}^{N} \left(\frac{m}{2} \dot{r}_{j}^{2} - \frac{m\Omega^{2}}{2} r_{j}^{2} \right) + \frac{m\omega^{2}}{2} \sum_{j,\ell>j}^{N} (\mathbf{r}_{j} - \mathbf{r}_{\ell})^{2}.$$
(22)

Introducing the center-of-mass and relative coordinates,

$$\mathbf{R} = \frac{1}{N} \sum_{j=1}^{N} \mathbf{r}_j, \tag{23}$$

$$\mathbf{x}_j = \mathbf{R} - \mathbf{r}_j, \tag{24}$$

¹For attractive interactions, BECs can become unstable especially in spherical geometries [46–48]. State-of-the-art experiments show that attractively interacting atomic BECs can nevertheless be stable on experimentally relevant time scales in quasi-one-dimensional waveguides [47–55]. While equivalent situations might be difficult to realize with photon BECs, as explained below Eq. (21), the reason why we focus on positive interactions for the LTI model is not a stability question: the grand-canonical partition function diverges. If there should be future experiments with attractively interacting photon condensates (for which there currently does not seem to be experimental evidence), this would require a more detailed modeling closer to the experiment.

the Lagrangian can be rewritten as

$$L(x_{j}, \dot{x}_{j}; R, \dot{R}) = \frac{Nm}{2} \dot{R}^{2} - \frac{Nm\Omega^{2}}{2} R^{2} + \sum_{j=1}^{N} \left(\frac{m}{2} \dot{x}_{j}^{2} - \frac{m(\Omega^{2} + N\omega^{2})}{2} x_{j}^{2} \right).$$
(25)

This new Lagrangian is of course subject to the constraint $\mathbf{R} = \frac{1}{N} \sum_{j=1}^{N} \mathbf{r}_{j}$, so although it looks as if it has N+1 degrees of freedom per spatial dimension, there are only N independent ones. Of these, one has eigenfrequency Ω and N-1 have eigenfrequency

$$w = \sqrt{\Omega^2 + N\omega^2}. (26)$$

Switching the sign of the last term in the Lagrangian turns the interactions from attractive to repulsive and leads to $w = \sqrt{\Omega^2 - N\omega^2}$. This means that for repulsive harmonic interactions, there is an upper bound to the number of particles that can be held together by the trap. In order for the grand-canonical ensemble to include all number states we therefore restrict ourselves to the case of attractive interactions. In contrast to the attractive contact potential, for a harmonic potential this does not lead to a collapse but rather to a change of the trapping frequency Ω to w for N-1 (D-dimensional) degrees of freedom. The remaining center-of-mass degrees of freedom acquire a frequency Ω . In a series of papers [42,43,62,63], Brosens, Devreese, and Lemmens explored this system and derive the canonical partition sum as follows:

$$Z_N(\beta, w) = \frac{\sinh^D(\beta \hbar w/2)}{\sinh^D(\beta \hbar \Omega/2)} \mathbb{Z}_N(w), \tag{27}$$

with

$$\mathbb{Z}_{N}(w) = \sum_{\substack{\{M_{1}, M_{2}, \dots, M_{N}\}\\ \sum \ell M_{\ell} = N}} \left(\prod_{\ell} \frac{\xi^{M_{\ell}(\ell-1)}}{M_{\ell}! \ell^{M_{\ell}}} \frac{1}{[2 \sinh(\ell \beta \hbar w/2)]^{2M_{\ell}}} \right).$$
(28)

Here D is the number of spatial dimensions, and $\xi = -1$ for fermions and $\xi = +1$ for bosons. The prefactor in front of \mathbb{Z}_N in expression (27) takes care of the center-of-mass degrees of freedom. The summation runs over all sets of natural numbers $\{M_1, M_2, \ldots, M_N\}$ satisfying the condition that $\sum_{\ell=1}^{\infty} \ell M_{\ell} = N$. This restriction makes the sum impossible to evaluate directly. However, it can be lifted by introducing the generating function

$$\mathcal{G}_0(u) = \sum_{n=0}^{\infty} u^n \mathbb{Z}_n(w). \tag{29}$$

The summation is taken while keeping w fixed. It is clear that $\mathbb{Z}_n(w)$ is the canonical partition function of n noninteracting identical particles in a harmonic confinement of frequency w. The generating function evaluates to

$$G_0(u) = \exp\left\{\xi \sum_{\ell=1}^{\infty} \frac{(\xi u b)^{\ell}}{\ell (1 - b^{\ell})^D}\right\},$$
 (30)

where

$$b = \exp\{-\beta \hbar w\}. \tag{31}$$

In order to retrieve \mathbb{Z}_N from $\mathcal{G}_0(u)$ one can use the formula

$$\mathbb{Z}_N = \frac{1}{N!} \frac{d^N \mathcal{G}_0}{du^N} \bigg|_{u=0}.$$
 (32)

This leads to a recursion formula as shown in Ref. [42],

$$\mathbb{Z}_N = \frac{1}{N} \sum_{m=0}^{N-1} \left(\frac{b^{(N-m)/2}}{1 - b^{N-m}} \right)^D \mathbb{Z}_m.$$
 (33)

In Appendix A we outline the algorithm we have implemented to generate the list of \mathbb{Z}_N 's from this recursion formula in a numerically stable way. We apply the BDL formalism for bosons ($\xi = 1$) in D = 2 dimensions [44].

It would be tempting to identify $\mathcal{G}_0(u)$ defined above with a grand-canonical partition function $\Xi(u)$ (up to the correction factor for the center-of-mass degree of freedom). As noted in Refs. [62,64], this is wrong. In the sum for the generating function $\mathcal{G}_0(u)$, the frequency w is kept fixed. However, the interactions change the spectrum, so systems with a different number of particles have a different basic frequency $\hbar w$ for the harmonic oscillator. This is typical for interacting systems: Adding more particles changes the effective single-particle levels. Indeed, mean-field shifts are an example of this. Usually, in defining the grand-canonical partition sum, this effect is ignored and one assumes that for large-enough numbers of particles, adding or removing a few particles only leads to negligible changes in the effective single-particle spectrum.

For smaller numbers of atoms this is clearly not true and it is necessary to go back to the original definition of the grand-canonical partition sum as an ensemble sum. Consider an open subsystem where interactions are present, and a reservoir (a large box of ideal gas) that can supply or remove particles from the subsystem. The grand-canonical partition sum is then

$$\Xi = \sum_{n} \sum_{E_s(n)} \exp\{-\beta [E_s(n) - \mu n]\}.$$
 (34)

Here the grand canonical ensemble of microstates of the entire system is subdivided into canonical ensembles where the subsystem has n particles. Each of these canonical ensembles can be further subdivided into microcanonical ensembles according to the possible energy states E_s of the subsystem. However, the list of possible energy states does not need to be the same for each canonical ensemble, so we have $E_s(n)$. In our example, the values of E_s are given by $\hbar w_n(\nu+1)$ with $\nu \in \mathbb{N}$ and $w_n = \sqrt{\Omega^2 + n\omega^2}$. The grand-canonical partition sum corresponding to (34) can be written as

$$\Xi(z) = \sum_{n=0}^{\infty} z^n Z_n(\beta, w_n). \tag{35}$$

Given the list of \mathbb{Z}_n 's, and a fixed $N = \langle n \rangle$, the fugacity z is found by numerically solving

$$\langle n \rangle = \frac{1}{\Xi(z)} \sum_{n=0}^{\infty} n z^n Z_n(\beta, w_n). \tag{36}$$

Note that, in general, not for every N a solution exists for z (for example, in fermionic systems with partially filled degenerate energy levels [64]). However, even in these cases the generating function formalism can still be used to calculate the exact canonical partition sums.

Although $\Xi(z)$ clearly differs from $G_0(u)$ defined above, there is a link. When the average number of particles in the subsystem $N = \langle n \rangle$ becomes large, and the temperature is above the condensation temperature for bosons, the summation above is sharply peaked around N. Only terms with $n \approx N$ contribute, so often one even approximates the sum by a single term, $\Xi(z) = z^N \mathbb{Z}_N(w_N)$, the saddle-point approximation. This approximation yields the well-known free-energy formula $\Omega(\mu) = F(N) - \mu N$. This formula is only true at the saddle-point level, as the neglected terms generate a correction term to it. However, it means that if N is large enough (and the temperature is above the critical temperature of condensation), then in the small range of relevant n's in the summation one may keep $w_n \approx w_N$ fixed. Only under these conditions $\Xi(z) \approx G_0(z)$. When the conditions are violated (for example, when studying condensate fluctuations at low temperatures), this is no longer true. This has a strong effect on the fluctuations $\Delta N = (\langle n^2 \rangle - \langle n \rangle^2)^{1/2}.$

III. RESULTS

A. Overview of Sec. III

In Sec. III B we use the fact that for very low temperatures, $k_B T \ll \hbar \omega$, the model of Ref. [35] introduced in Sec. II C becomes exact to make analytical predictions for the size of the fluctuations at low temperatures.

Temperatures are given in units of the condensation temperature of a noninteracting Bose gas in a two-dimensional harmonic oscillator (in the version which can be found, e.g., in Ref. [29] and references therein)

$$k_B T_0 \equiv \hbar \omega \frac{\sqrt{6}\sqrt{\langle n \rangle}}{\pi}.$$
 (37)

Both for the total number fluctuations (Sec. III B) and for condensate fluctuations (Sec. III C) as well as for the kurtosis (Sec. III D) the qualitative statements of the BDL model agree with the fundamentally different LTI model: On the one hand, for temperature $T \gtrsim T_0$, a weakly interacting grand-canonical BEC essentially behaves like a noninteracting grand-canonical BEC. On the other hand, for low temperatures the deviations are very large—the weakly interacting grand-canonical BEC behaves more like a canonical BEC.

B. Total number fluctuations within the grand-canonical ensemble

The LTI model allows to derive analytical results for the total number fluctuations for very low temperatures ($k_BT \ll \hbar\omega$; exp($-\beta\hbar\omega$) \ll 1). In this limit, Eq. (14) simplifies to

$$Z_N^{(ex)}(\beta) \simeq 0, \quad N > 0. \tag{38}$$

Furthermore, Eq. (17) becomes

$$Z_N(\beta) \simeq \exp[-\beta \alpha N(N-1)],$$
 (39)

and Eq. (19) now reads

$$\Xi(\beta) \simeq \sum_{n=1}^{\infty} z^n \exp[-\beta \alpha n(n-1)], \tag{40}$$

$$\simeq \int_{-\infty}^{\infty} dn z^n \exp[-\beta \alpha n(n-1)], \tag{41}$$

$$= \frac{\sqrt{\pi}}{\sqrt{\beta\alpha}} \exp\left(\frac{1}{4} \frac{(\ln(z) + \beta\alpha)^2}{\beta\alpha}\right). \tag{42}$$

This analytical result can be used to obtain

$$\langle n \rangle = -z \frac{\partial}{\partial z} \ln[\Xi(\beta)],$$
 (43)

$$= -1/2 - \frac{\ln(z)}{2\beta\alpha},\tag{44}$$

and, in particular,

$$\langle \Delta n^2 \rangle = z \frac{\partial}{\partial z} z \frac{\partial}{\partial z} \ln[\Xi(\beta)],$$
 (45)

$$=\frac{k_B T}{2\alpha}. (46)$$

Thus, in the limit $k_B T \lesssim \alpha \ll \hbar \omega$, the variance of the total number of particles is independent of $\langle n \rangle$ and goes to zero. This implies that canonical and grand-canonical ensembles become equivalent again. Therefore, the we predict that the grand-canonical condensate fluctuations vanish when the temperature goes to zero.

The limit $\alpha \to 0$ has to be taken with care in Eq. (46): The fact that the relative fluctuations $\Delta n/\langle n \rangle$ seem to diverge only signifies that the approximation (41) breaks down.

However, as long as $k_B T \ll \hbar \omega$, $\Delta n/\langle n \rangle < 1$ and $T < T_0$, $\langle n \rangle (\langle n \rangle - 1)\alpha < \hbar \omega$ the fluctuations of the total number of bosons is given by Eq. (46).

While the analytical result of Eq. (46) can only be valid for low temperatures, in this temperature regime it agrees well with the full numerical results within the LTI model shown in Fig. 1. In order for the model to be consistent, we choose interactions that are weak in the sense that the sums in Eq. (2) have converged at $N \approx N_{\rm max}/2$ and $E_0(N_{\rm max}/2) \lessapprox \hbar \omega$.

To show the effect of interactions in the BDL model, we choose a grand-canonical ensemble where the average number of particles is fixed at $\langle n \rangle = 100$. Taking $\omega = 0.01$ for the interaction strength (and $\Omega = 1$ as energy unit), we use the number-dependent frequency $w_n = \sqrt{\Omega^2 + n\omega^2}$ to calculate the expectation value $\langle n^2 \rangle$, and the corresponding ΔN . For the corresponding noninteracting case, we use the number-independent value w_{100} for the frequency at any n. If the sums are very sharply peaked around n = 100, then the effect of the interactions on the fluctuations will hence be small. However, if the sums broaden out and many terms need to be taken into account to get the total, then there will be a significant difference. So we expect that for higher temperatures, both results will coincide, whereas for temperatures below the condensation temperature, differences may occur. The results are shown in Fig. 2. For the temperature unit we use $T_0 = \hbar w_{100} \sqrt{6 \times 100} / (\pi k_B) = 7.797 \ \hbar w_{100} / k_B$. At large temperatures, the fluctuations tend to $\Delta N = \sqrt{N}$, as one expects in the classical limit [this is indicated by a

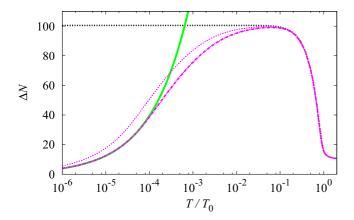


FIG. 1. The fluctuation ΔN in the total number of particles in the subsystem within the LTI model. Thick magenta (dark gray) dash-dotted curve: grand canonical ensemble $N_{\rm max}=2000$, $\langle N \rangle=100$, $\alpha=1/4\,000\,000$. For very low temperatures, this agrees with the analytic prediction (46) [green (light gray) solid curve] and for higher temperatures with the noninteracting grand-canonical ensemble [(black) dashed curve]. Thin magenta (dark gray) dashed curve: grand canonical ensemble for the same parameters as the thick dash-dotted curve except for a reduced $\alpha=1/8\,000\,000$. For both interaction parameters predictions of all three versions of the LTI model are plotted; the data lie on top of each other.

horizontal line at $\Delta N=10$ in the figure]. When no interactions are present (dashed black curve), the grand-canonical fluctuations on the total number tend to $\Delta N=\sqrt{N(N+1)}$ as the temperature goes to zero (there is a horizontal line at $\Delta N=100$ in the figure). When interactions are present, this reduces the grand-canonical fluctuations for temperatures below T_0 . Nevertheless, there is an intermediate regime where the fluctuations are still substantial, reaching $\Delta N\approx 70$ of N=100 particles. In the absence of strong correlations, the fluctuation in the number of particles in any given energy

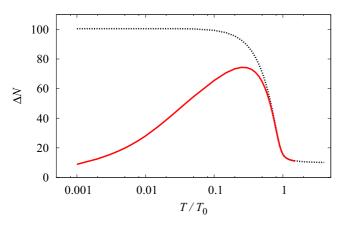


FIG. 2. The fluctuation ΔN in the total number of particles in the subsystem within the BDL model, the grand-canonical ensemble is plotted here as a function of temperature. The chemical potential is set such that the average number of particles in the subsystem is $\langle n \rangle = 100$. The temperature unit is $T_0 = \hbar w_{100} \sqrt{6 \times 100}/\pi$, where $w_{100} = \sqrt{\Omega^2 + 100}\omega^2$ and $\Omega = 1, \omega = 0.01$. The dashed black curve keeps $w = w_{100}$ constant, and the full red (black) curve takes into account interactions and uses w_n .

level should be smaller than the fluctuation in the total number of particles. In particular, we expect that the fluctuation in the condensate number is bound by ΔN . Hence, interactions also prevent grand-canonical condensate fluctuations from becoming as large as the total number of particles.

C. Condensate number fluctuations

For our investigation of the condensate number fluctuations, we start with numerical results obtained within the BDL model. Using again $\langle n \rangle = 100$ to fix z, we can now calculate the grand-canonical expectation value for the number of condensate atoms as

$$\langle n_0 \rangle^{\text{gc}} = \frac{1}{\Xi(z)} \sum_{n=0}^{\infty} \langle n_0 \rangle_n^{\text{can}} z^n Z_n(\beta, w_n). \tag{47}$$

Here, $\langle n_0 \rangle_n^{\rm can}$ is the expectation value of the number of condensate atoms in the *canonical* ensemble with n particles, and $\Xi(z)$ is given by expression (35). Within the BDL model, the canonical condensate number can be expressed as a recursion relation [42], as outlined in Appendix B. The algorithm for computing the recursion relation is outlined in Appendix A. Similarly, $\langle n_0^2 \rangle_n^{\rm can}$ can be computed and used to find $\langle n_0^2 \rangle_n^{\rm gc}$, allowing us to find the grand-canonical fluctuations for the number of condensate atoms,

$$(\Delta n_0)^{\text{gc}} = \sqrt{\langle n_0^2 \rangle^{\text{gc}} - (\langle n_0 \rangle^{\text{gc}})^2}.$$
 (48)

As before, to switch off the effects of interaction, we work at a fixed frequency w_{100} rather than an n-dependent frequency.

The results are shown in Figs. 3 and 4. Figure 3 shows that, in the BDL model as well, the stronger the interactions, the lower the fluctuations. In Fig. 4 three cases are compared: (a) the canonical ensemble for 100 particles, (b) the grand-canonical ensemble without interactions [with $\langle n \rangle = 100$], and (c) the grand-canonical ensemble with interactions ($\omega = 0.01$ and again $\langle n \rangle = 100$). The dashed line shows the result for the condensate number, closely equal in all three cases, and showing some finite-number effects when compared to the

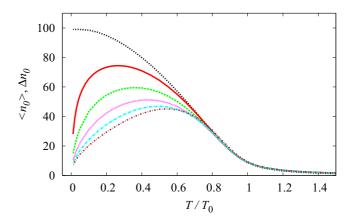


FIG. 3. The statement that the stronger the interaction the smaller are interactions is also true in the BDL model. The top curve shows the condensate fraction, and all other curves show the condensate fluctuations for (from top to bottom): $\omega = 0.01, 0.02, 0.03, 0.04$, and 0.05.

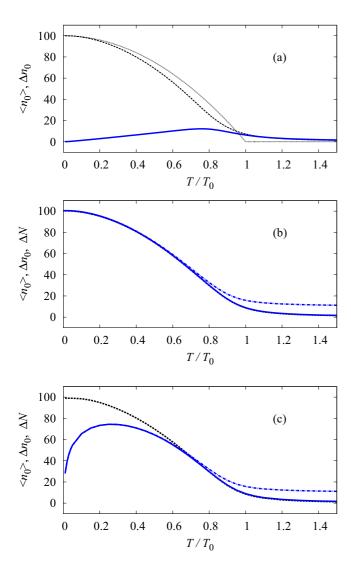


FIG. 4. In each panel, results within the BDL model are plotted as a function of temperature. The dashed black line shows the number of condensate atoms n_0 and the full blue line shows the fluctuation Δn_0 of this condensate number; both are plotted as a function of temperature. The top panel shows the result in the canonical ensemble with 100 particles. The middle panel shows the results in the grand-canonical ensemble; for the case without interactions, the fluctuations are as large as the condensate number. The bottom panel illustrates the effect of interactions ($\omega=0.01$ in the model) on the grand-canonical fluctuations. The dotted black line in panel (a) shows the result for n_0 in the thermodynamic limit. The dash-dotted blue (black) line in the bottom two panels shows the fluctuations for the total number of particles in the grand-canonical ensemble.

result in the thermodynamic limit [dotted line in Fig. 4(a)]. The full line shows the condensate fluctuations as a function of temperature, and for this quantity it is clear that the results strongly differ. In the canonical ensemble, fluctuations remain small and are only weakly enhanced close to the critical temperature. Without interactions, in Fig. 4(b), it is apparent that the condensate fluctuations are as large as the condensate number. Interactions suppress the grand-canonical fluctuations at low-enough temperature: In Fig. 4(c) the fluctuations decrease when the temperature dips below $0.3T_0$. Numerical

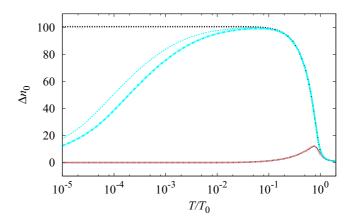


FIG. 5. The condensate number fluctuation Δn_0 within the LTI model. Thick light blue (light gray) dash-dotted curve: grand canonical ensemble $N_{\rm max}=2000, \langle N\rangle=100, \alpha=1/4\,000\,000$. For higher temperatures, this again agrees with the non-interacting grand-canonical predictions (black dashed curve). As for the fluctuations of the total number, for lower temperature the system behaves more like a canonical ensemble [black (brown) dotted curves] for which interacting and noninteracting curves lie on top of each other. Thin light blue (light gray) dashed curve: Decreasing the interaction in the grand canonical enesmble by a factor of 2 again shifts the curve toward higher fluctuations (cf. Fig. 1). As in Fig. 1, the predictions of all three versions or the LTI model lie on top of each other.

inaccuracy prevents computation of the T=0 results, so the lowest temperature shown is T=0.01. The dash-dotted curve in Figs. 4(b) and 4(c) shows the grand-canonical fluctuation for the total number of particles. Below the condensation temperature, the fluctuation in total number is dominated by the contribution of the condensate fluctuations. Near the critical temperature and above it, the condensate fluctuations dip below the fluctuation in the total number of atoms, as expected. At high temperatures, the standard square-root fluctuations are retrieved. From Fig. 4(c) it is also clear that interactions suppress both fluctuations in the total number of particles but also condensate fluctuations.

The LTI model again yields results that are qualitatively very similar to those of the BDL model. Figure 5 displays the condensate fluctuations within the LTI model. Although this model considerably differs from the BDL model, the qualitative statements about the behavior at low and high temperatures are the same as in the BDL model (Fig. 4): For low temperatures, interaction dramatically changes the condensate fluctuations to a behavior close to the canonical ensemble: The condensate fluctuations vanish at low temperatures (as was to be expected from the vanishing fluctuations in the total number of photons, cf. Figs. 1 and 2).

D. Kurtosis and non-Gaussian fluctuations of the total number of particles

The "classical" fluctuations of the total number of atoms in an open subsystem are Gaussian, with a width equal to \sqrt{N} . When the temperature of a Bose gas drops below the critical temperature, these fluctuations increase strongly, and the standard deviation becomes as large as the total number of particles, $\sqrt{N(N+1)}$. Does this correspond to a

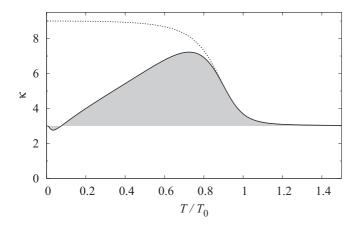


FIG. 6. Kurtosis (49) of the total number fluctuation distribution in the grand-canonical ensemble with the BDL model as a function of temperature and for $\langle n \rangle = 100$. The full line is for the case with interactions ($\omega = 0.01$), whereas the dashed line is for the ideal gas. The value $\kappa = 3$ would correspond to Gaussian fluctuations; it is highlighted via the shaded region.

wider Gaussian or do the fluctuations obtain a non-Gaussian character? A widely used (see, e.g., Refs. [19,65–67] and references therein) quantifier of non-Gaussianity is the excess kurtosis, $\gamma = \kappa - 3$ with the kurtosis itself defined by

$$\kappa = \frac{\langle (n-N)^4 \rangle}{(\Delta N)^4},\tag{49}$$

i.e., the ratio of the fourth central moment to the second central moment squared. Here again $N = \langle n \rangle$ and $(\Delta N)^2 =$ $\langle (n-N)^2 \rangle$. For a Gaussian distribution, $\kappa = 3$. There exist other methods to measure non-Gaussianity (for example, the entropy) that are less sensitive to outliers, but the kurtosis is very easy to calculate in the present treatment, since we can compute any moment $\langle n^p \rangle^{\rm gc}$ of the grand-canonical number distribution (as outlined in Appendix B). The excess kurtosis can be determined by repeated measurement of the number and building up statistics to estimate the second and fourth moments. Applications in other fields, for example, detecting "fat tails" in the velocity distributions of turbulent fluids [65] or in time series of financial instruments [68], show that using the fourth moment to estimate the non-Gaussian nature of the distribution is robust to other sources of noise and more accessible than, for example, Castaign's measure [69].

Figure 6 shows the result for κ as a function of temperature. For the thermal Bose gas, at temperatures above T_0 , the fluctuations are indeed Gaussian and $\kappa=3$. Excess kurtosis appears below T_c , indicating a more "peaked" distribution with a "fatter tail." When no interactions are present, this excess kurtosis remains present as the temperature is lowered to zero. Including interactions ($\omega=0.01$ as before) is seen to reduce the kurtosis back down to 3 as the temperature goes to zero. So interactions not only suppress the size of the fluctuations, they also tend to keep the fluctuations Gaussian. This effect is more pronounced at temperatures well below T_0 . When the temperature is near to T_0 the effect of the interactions is less. Note that there is a small leptokurtic region at temperatures just above zero—it is not clear whether this is an artifact of

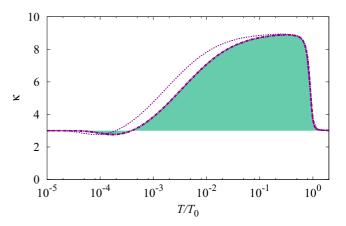


FIG. 7. Thick dash-dotted purple (black) line: Kurtosis (49) of the total number fluctuation distribution in the grand-canonical ensemble with the LTI model. The shaded green (black) area indicates if the kurtosis lies above or below the result for Gaussian fluctuations. Interaction parameters as in Fig. 1; the thin dashed purple (black) line again represents the parameters for which the interaction has been decreased by a factor of 2; for very low temperatures this decreases the kurtosis, and for larger temperatures it increases the kurtosis. Qualitatively, the LTI model again predicts a behavior similar to the BDL model (Fig. 6). As in Figs. 1 and 5, the predictions of all three versions or the LTI model lie on top of each other.

the calculations (we take n up to 2000 for the sum in the grand-canonical ensemble) or whether this is real.

The LTI model (Fig. 7) again predicts a behavior that is qualitatively very similar to that of the BDL model (Fig. 6).

IV. CONCLUSION

Motivated by the landmark experiment observing grand-canonical statistics in photon condensates [16], we revisit differences between statistical ensembles when describing Bose-Einstein condensates. The focus of the current paper lies in microscopic modeling of thermodynamic properties for small but experimentally accessible particle numbers. For an ideal Bose gas the grand-canonical ensemble predicts rms fluctuations for both the total number of particles and for the number of particles in the condensate that are larger than the average number of particles (see Figs. 1, 2, and 5). While this clearly is unphysical for an atomic Bose-Einstein condensate with constant atom numbers, photon condensates open an entirely new world by making highly fluctuating total photon numbers possible.

However, the realization of a grand-canonical photon condensate does not automatically imply that the textbook treatment of an ideal gas is valid. Thus, we model *weakly interacting* photon condensates in order to investigate both condensate fluctuations and fluctuations of the total number of particles in the exactly solvable BDL model [42,43] and in the LTI model based on Ref. [35]. The latter model becomes exact in the limit of low temperatures for pairwise interactions. As our two models fundamentally differ from each other, this helps us to identify model-independent properties of, for example, fluctuations of the total number of particles.

Our paper focuses on a grand-canonical Bose gas interactions that are so weak that the canonical fluctuations (for fixed total particle numbers) match well the results for a noninteracting system of bosons. The main results are listed below:

- (1) In the recent experiment of Ref. [16] it is mentioned that the statistics can be influenced by changing the effective size of the reservoir by changing the number of dye molecules. However, as in the variational treatment of Ref. [45], our microscopic treatment finds that already weak interaction changes the fluctuations dramatically for low temperatures: Rather than $(\Delta N_0^2) \sim (N_0)^2$ as predicted for the ideal gas, the grand-canonical fluctuations vanish at low temperatures.
- (2) The interactions come into play essentially when we move to the grand-canonical ensemble. Thus, the textbook example for treating Bose-Einstein condensation, the ideal Bose gas, is a too-idealized example to correctly describe the grand-canonical fluctuations investigated experimentally in Ref. [16]. Slightly below the condensation temperature, we still find very large rms fluctuations $\propto N$. As our paper focuses on experimentally realistic small particle numbers, this is very distinct from considerations arguing against the existence of anomalous fluctuations based on stability arguments in the thermodynamic limit [38,39]. However, in agreement with Refs. [38,39], even very weak interactions considerably suppress fluctuations.
- (3) We find that the *fluctuations are strongly non-Gaussian*, *showing substantial excess kurtosis*. For low temperatures, even very weak interactions suppress both fluctuations and the non-Gaussian character of the fluctuations.

For the BDL model, the fact that the center-of-mass degree of freedom may have a frequency that differs from all the other degrees of freedom does not alter the number of condensate particles or the condensate fluctuation. When no interactions are present, it is known that the condensate fluctuations in the grand-canonical ensemble become as large as the total number of particles.

In the BDL model considered here, the role of interactions is to change the spectrum of possible energy states of the subsystem as a function of the number of particles in the subsystem. There is a secondary effect of interactions, clear in the transition from \mathbb{Z}_N to Z_N , which consists of endowing one degree of freedom with frequency Ω rather than w_N . However, this single degree of freedom has only a negligible effect on the results, even for $\langle n \rangle$ as low as 100—whether we work with \mathbb{Z}_N or Z_N , we find qualitatively the same results. These results for the harmonically interacting model system show that interactions reduce the number fluctuations in the grand-canonical ensemble and make the fluctuations more Gaussian.

The data presented in this paper will be available soon on https://collections.durham.ac.uk/files/vt150j289 and http://dx.doi.org/10.15128/vt150j289 [70].

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APPENDIX A: EFFICIENT RECURSION ALGORITHMS FOR BDL

Retrieving $\mathbb{Z}(N)$ from $\mathcal{G}_0(u)$ leads to the following recursion formula, as derived in Ref. [42]:

$$\mathbb{Z}_N = \frac{1}{N} \sum_{m=0}^{N-1} \xi^{N-m-1} \left(\frac{b^{(N-m)/2}}{1 - b^{N-m}} \right)^D \mathbb{Z}_m, \tag{A1}$$

with $\xi=1$ for bosons and $\xi=-1$ for fermions, in D dimensions, and with $b=e^{-\beta\hbar w}$. Note that $\mathbb{Z}_0=1$ and

$$\mathbb{Z}_1 = \left[2\sinh(\beta\hbar w/2)\right]^{-D}.\tag{A2}$$

Straightforwardly implementing the recursion formula leads to large numerical inaccuracies. For bosons, there is a numerically fast and stable algorithm for evaluating it, as communicated to one of us (J.T.) by F. Brosens. We are not aware of it being described in detail in other publications, although it is mentioned in Ref. [43], where it is used to calculate the density and pair correlation in the 3D Bose gas. To facilitate reproducing our results, we include the description of the algorithm in this Appendix.

The recurrence relation is recast in a numerically more stable form by introducing new quantities $\mathfrak{z}(j)$ (for j = 1, ..., N) defined by

$$\mathbb{Z}_{N} = \prod_{j=1}^{N} \mathfrak{z}(j) \left(\frac{b^{1/2}}{1 - b^{j}} \right)^{D}, \tag{A3}$$

where by definition $\mathfrak{z}(1)=1$. Introducing the above representation of \mathbb{Z} in the recurrence relation (A1) and isolating $\mathfrak{z}(N)$ yields

$$\mathfrak{Z}(N) = \frac{1}{N} \sum_{m=0}^{N-1} \frac{(1-b^N)^D}{(1-b^{N-m})^D} \prod_{i=m+1}^{N-1} \frac{(1-b^j)^D}{\mathfrak{Z}(j)}.$$
 (A4)

Once the list of $\mathfrak{z}(j)$'s is found, we can find

$$\ln(\mathbb{Z}_N) = \sum_{i=1}^N \left[D \ln\left(\frac{b^{1/2}}{1 - b^j}\right) + \ln[\mathfrak{z}(j)] \right], \quad (A5)$$

which in turn leads to a recursion relation for the $ln(\mathbb{Z})$'s:

$$\ln(\mathbb{Z}_N) = D \ln\left(\frac{b^{1/2}}{1 - b^N}\right) + \ln[\mathfrak{z}(N)] + \ln[\mathbb{Z}_{N-1}], \quad (A6)$$

where we start with $\ln [\mathbb{Z}_0] = 0$, and since $\mathfrak{z}(1) = 1$, $\ln [\mathbb{Z}_1] = D \ln [b^{1/2}/(1-b)]$. Note that this recursive formula will yield the list $\mathbb{Z}_m(w)$ for a fixed w. Expression (A4) is implemented through succesive mul-

tiplications and additions, by the following algorithm which calculates $\mathfrak{z}(N)$ given $\mathfrak{z}(1), \ldots, \mathfrak{z}(N-1)$:

start with
$$\left(\frac{1-b}{1-b^N}\right)^D$$
, multiply by $\frac{(1-b)^D}{\mathfrak{z}(1)}$ and add $\left(\frac{1-b}{1-b^{N-1}}\right)^D$, multiply by $\frac{(1-b^2)^D}{\mathfrak{z}(2)}$ and add $\left(\frac{1-b}{1-b^{N-2}}\right)^D$, ... multiply by $\frac{(1-b^{N-2})^D}{\mathfrak{z}(N-2)}$ and add $\left(\frac{1-b}{1-b^2}\right)^D$ multiply by $\frac{(1-b^{N-1})^D}{\mathfrak{z}(N-1)}$ and add 1, divide by $N\left(\frac{1-b}{1-b^N}\right)^D$.

Note that for every N we need to perform the entire algorithm: We have not found a way to obtain $\mathfrak{z}(N)$ with less than $\mathcal{O}(N)$ additions and multiplications. The algorithm works for N > 1 and should be started with $\mathfrak{z}(1) = 1$.

A similar algorithm can be found for canonical expectation values that can be written as

$$\mathbb{E}[f] = \sum_{m=0}^{N} f(m) \frac{\mathbb{Z}_m}{\mathbb{Z}_N}.$$
 (A8)

Both the expression for $\langle n_0 \rangle_N^{\rm can}$ and that for $\langle n_0^2 \rangle_N^{\rm can}$ are of this form (see Appendix B). Then we rewrite the above using the product form (A3):

$$\frac{\mathbb{Z}_m}{\mathbb{Z}_N} = \prod_{j=m+1}^N \frac{1}{\mathfrak{z}(j)} \left(\frac{1 - b^j}{b^{1/2}} \right)^D.$$
 (A9)

Thus, we have

$$\mathbb{E}[f] = f(N) + \sum_{m=1}^{N-1} f(m) \prod_{j=m+1}^{N} \frac{1}{\mathfrak{z}(j)} \left(\frac{1-b^j}{b^{1/2}}\right)^D + \frac{f(0)}{\mathbb{Z}_N}.$$
(A10)

This can again be written as a series of summations and multiplications:

start with
$$f(0)$$
, multiply with $\frac{1}{\mathfrak{z}(1)} \left(\frac{1-b}{b^{1/2}}\right)^D$ and add $f(1)$, multiply with $\frac{1}{\mathfrak{z}(2)} \left(\frac{1-b^2}{b^{1/2}}\right)^D$ and add $f(2)$, ... multiply with $\frac{1}{\mathfrak{z}(N)} \left(\frac{1-b^N}{b^{1/2}}\right)^D$ and add $f(N)$.

This avoids the calculation of the canonical partition sums altogether. All we need is the list of $\mathfrak{z}(j)$'s obtained from (A4) with the algorithm (A7).

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APPENDIX B: CANONICAL CONDENSATE FLUCTUATIONS IN BDL

To calculate fluctuations of the number of atoms in the condensate, n_0 , we need to find the expectation value of n_0^p with $p \leq 2$, i.e., the first and second moments of the distribution. To find these, we again use a generating function approach, introducing

$$\mathcal{G}_p(u) = \sum_{n=0}^{\infty} \langle n_0^p \rangle_n^{\text{can}} u^n \mathbb{Z}_n.$$
 (B1)

Here $\langle ... \rangle_N^{\text{can}}$ denotes the expectation value in the canonical ensemble for N particles. This evaluates to $\mathcal{G}_p(u) = f_p(ub)\mathcal{G}_0(u)$ with

$$f_p(ub) = (1 - ub) \sum_{m=0}^{\infty} m^p (ub)^m.$$
 (B2)

For p = 1,2 this simplifies to

$$\mathcal{G}_1(u) = \frac{ub}{1 - ub} \mathcal{G}_0(u), \tag{B3}$$

$$G_2(u) = \frac{ub(1+ub)}{(1-ub)^2}G_0(u).$$
 (B4)

The expectation values are then extracted from the generating functions by applying the same technique as outlined in Ref. [42] for the partition functions, namely through writing out

$$\langle n_0^p \rangle_N^{\text{can}} = \frac{1}{\mathbb{Z}_N} \frac{1}{N!} \frac{d^N \mathcal{G}_p(u)}{du^N} \bigg|_{u=0}$$
 (B5)

by recursively applying the derivative with respect to u. This yields

$$\frac{d^{N}\mathcal{G}_{p}(u)}{du^{N}}\bigg|_{u=0} = \sum_{\ell=0}^{N} \frac{N!}{\ell!} \frac{d^{\ell}[f_{p}(ub)]}{du^{\ell}}\bigg|_{u=0} \mathbb{Z}_{N-\ell}, \quad (B6)$$

from which

$$\langle n_0^p \rangle_N^{\text{can}} = \sum_{\ell=0}^N \frac{1}{\ell!} \frac{d^\ell [f_p(ub)]}{du^\ell} \bigg|_{u=0} \frac{\mathbb{Z}_{N-\ell}}{\mathbb{Z}_N}.$$
 (B7)

In particular, for p = 1 and 2 we obtain

$$\langle n_0 \rangle_N^{\text{can}} = \sum_{\ell=1}^N \frac{b^\ell \mathbb{Z}_{N-\ell}(w)}{\mathbb{Z}_N(w)}$$
 (B8)

and

$$\langle n_0^2 \rangle_N^{\text{can}} = \sum_{\ell=0}^N \frac{(2\ell-1)_+ b^\ell \mathbb{Z}_{N-\ell}}{\mathbb{Z}_N},$$
 (B9)

where $(a)_+ = \max[a,0]$. From these moments we get the condensate fluctuations through

$$(\Delta n_0)^{\text{can}} = \sqrt{\langle n_0^2 \rangle_N^{\text{can}} - \left(\langle n_0 \rangle_N^{\text{can}} \right)^2}.$$
 (B10)

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