Hybrid Metropolis Approach to BEC Fluctuations

M. B. Kruk[1,2], K. Pawłowski[1], D. Hryniuk[1], P. Kulik[1], K. Rzążewski[1]

[1] *Center for Theoretical Physics, Polish Academy of Sciences, Aleja Lotników 32/46, 02-668 Warsaw, Poland*
[2] *Institute of Physics, Polish Academy of Sciences, Aleja Lotników 32/46, 02-668 Warsaw, Poland*

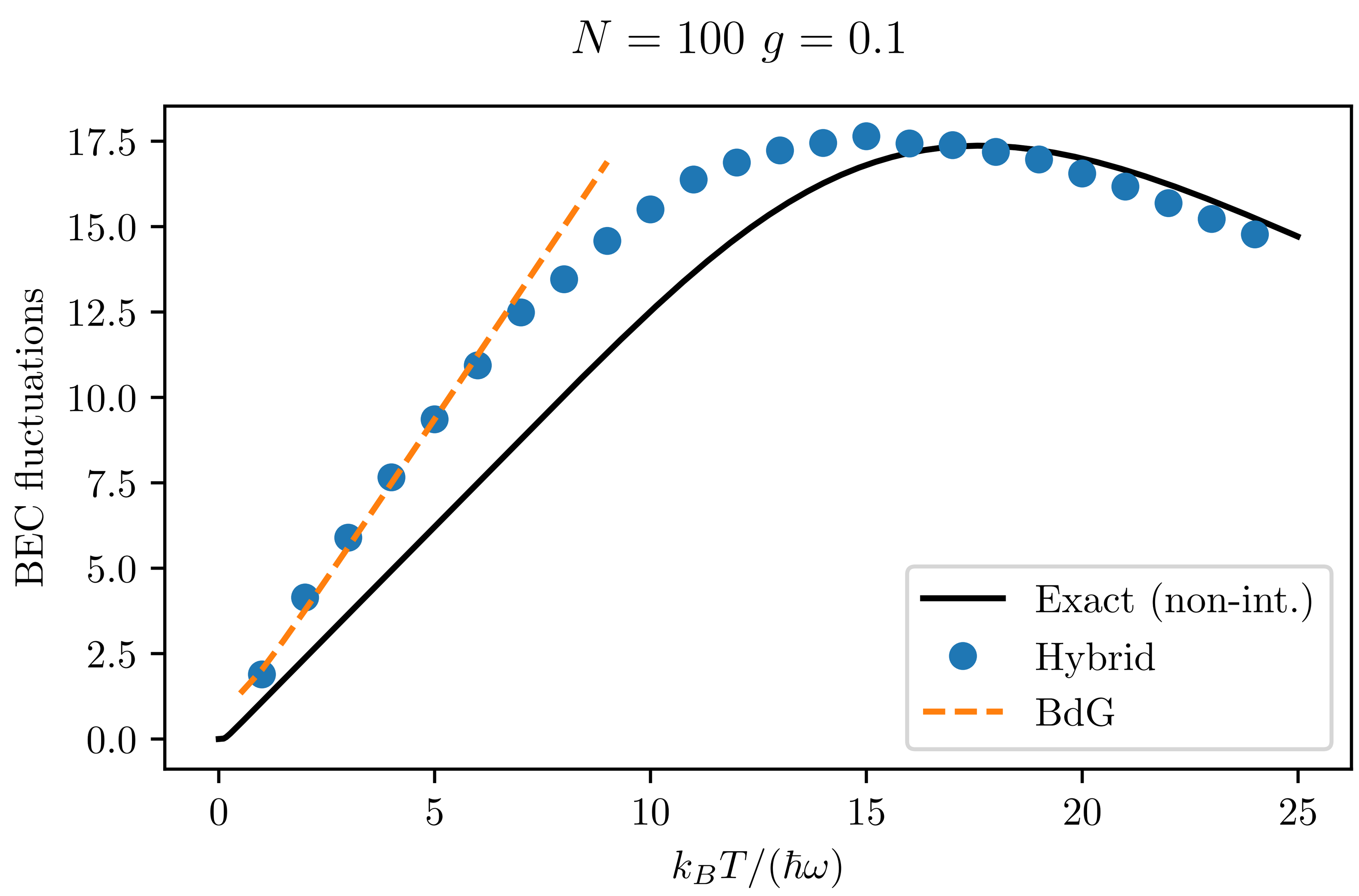
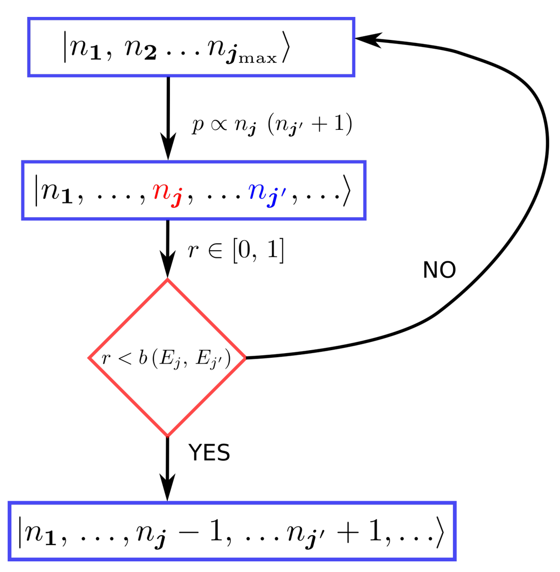


Figure 1: Condensate in the canonical ensemble, in a 1D harmonic potential trap. New hybrid approach shows excellent agreement compared with Bogoliubov approximation.

1 The method

Fock State Sampling (FSS) is a new method for calculating BEC fluctuations developed by our group, which was already put to the test in [1]. It is essentially a Metropolis algorithm that samples multimode Fock state configurations in a chosen statistical ensemble, with an innovative update rule that deals efficiently with the high energy tails.



Single step of the FSS method: one draws two states – one from which an atom might be taken (index $\boldsymbol{j}$) and one in which the atom may land (index $\boldsymbol{j'}$) with probability distribution proportional to $n_j\,(n_{j'}+1)$. The new state is accepted only if a random number r drawn from a uniform distribution in [0, 1] is smaller than the Boltzman factor $b\,(E_{current}, E_{candidate}) = \exp\left(-\beta\,(E_{current} - E_{candidate})\right)$.

In the interacting case with general hamiltonian

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \frac{g}{2}\int \hat{\Psi}(x)^\dagger\hat{\Psi}(x)^\dagger\hat{\Psi}(x)\hat{\Psi}(x)\mathrm{d}x,$$

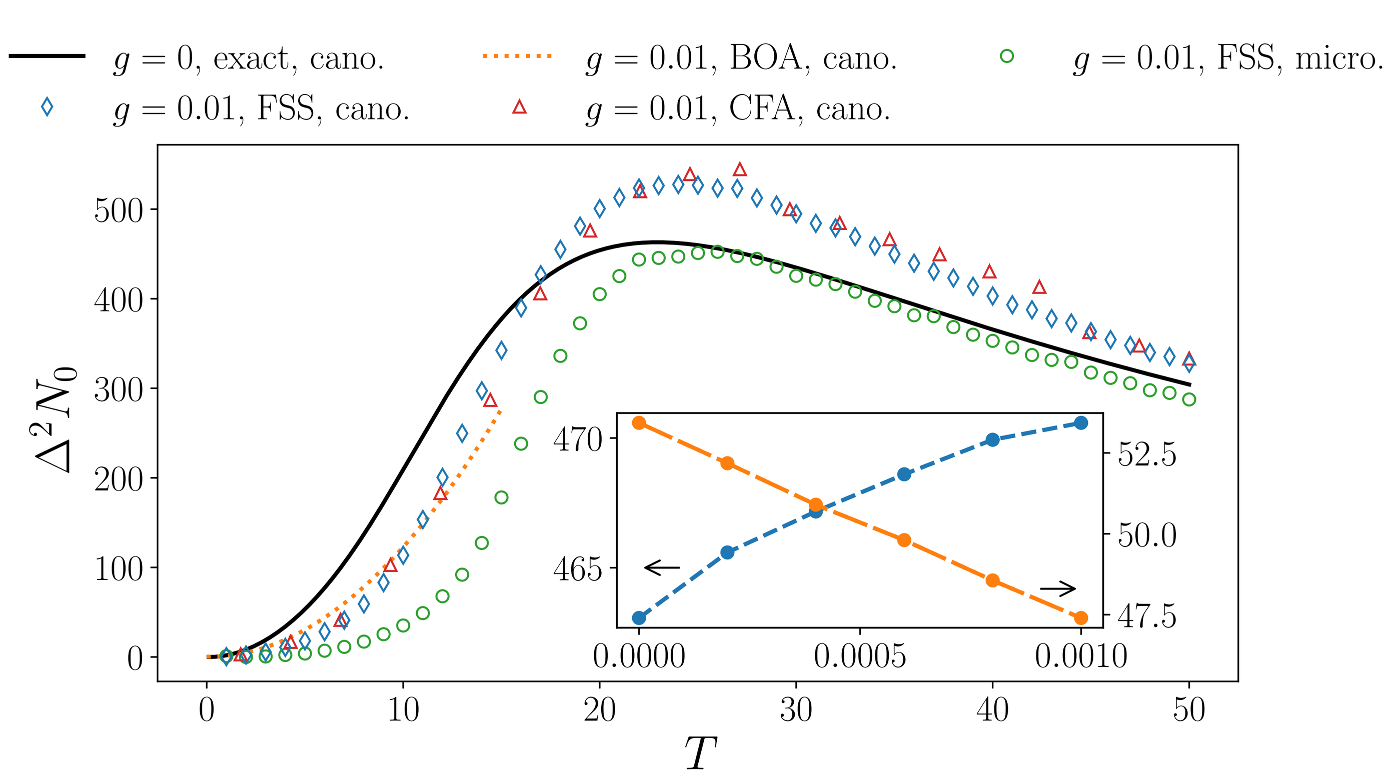
where $\hat{\Psi}(x) = \Sigma_i\,\psi_i(x)\hat{a}_i$ are the field operators constructed from annihilation operators $\hat{a}_i$ and the corresponding $\psi_i(x)$ single particle eigenfunctions ("orbitals") of the non-interacting Hamiltonian $\hat{\mathcal{H}}_0$. $\psi_i(x)$ form an orthonormal basis on the underlying single particle Hilbert space.

To compute the candidate's energy the following perturbative approximation is used:

$$E = \langle\phi|\hat{\mathcal{H}}|\phi\rangle = \sum_i E_i n_i + \frac{g}{2}\sum_i h_{ii}(n_i - 1)n_i + 2g\sum_{i<j} h_{ij} n_i n_j$$

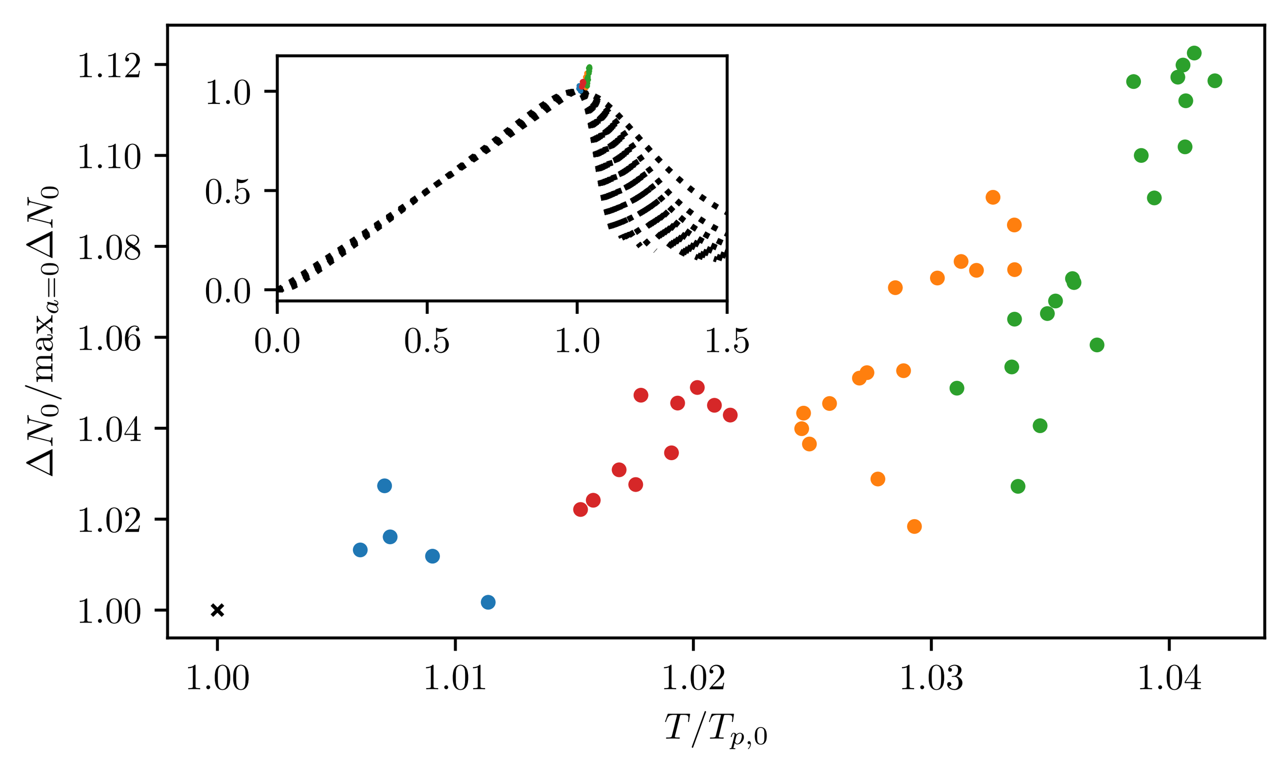
where ϕ are the eigenstates of $\hat{\mathcal{H}}_0$ which allows for efficient computation of ΔE once the overlaps h_{ij} have been pre-computed.

2 Microcanonical vs Canonical Fluctuations in a 1D box [2]



Fluctuations of a weakly-interacting Bose gas containing $N = 100$ atoms in a 1D ring trap. The variance of N_0 as a function of temperature is obtained from several different approaches: FSS method, classical field approximation, and Bogoliubov approach. A microcanonical calculation shows a significant suppression of the fluctuations. (inset) Variance at a low temperature $T = 5$ (orange, axis on the right) and at the temperature of maximal fluctuations (blue, axis on the left) as a function of the interaction strength g, obtained with the FSS method in the canonical ensemble. The arrows indicate the appropriate axis.

3 Characteristic temperature shift in a 3D box [3]



Relative standard deviation of the BEC atom number for an interacting gas (coloured points) for various total numbers of atoms, and interaction strengths. All points are rescaled by the maximal value of the fluctuations in the non-interacting case. Results for systems with the same gas parameter are marked with the same colour, i.e. $a\rho^{\frac{1}{3}}$ corresponds to 0.005 (blue), 0.01 (red), 0.015 (orange), 0.02 (green) . The quantity $T_{p,0}$ is the temperature of maximal fluctuations of the non-interacting gas and the symbol "X" marks the reference point – the maximal BEC fluctuations of the non-interacting gas. The atom number is in the range $N = 100, 200, ..., 1000, 2000, ..., 10000$. The inset shows an overview of the entire temperature range with the results for the non-interacting gas (dashed lines). We obtain the relative characteristic temperature shift:

$$\delta T_{\rm p} \approx (2.039 \pm 0.014)\left(a\rho^{1/3}\right), \tag{1}$$

4 Hybrid approach

Classical fields approximation: has superpositions but suffers from UV divergency (cutoff problem).
Fock State Sampling: no cutoff problem but lacks orbital superpositions.

Let's combine advantages of both methods and introduce an effective field: $\phi(x) = \Sigma_i\,\alpha_i\psi_i(x)$, where $\alpha_i \in \mathbb{C}$ and $|\alpha_i|^2 = n_i \in \mathbb{Z}_+$ are discrete occupations of orbitals that also encode relative phases between them. In hybrid approach we change energy evaluation method the one inspired by classical fields:

$$E = \sum_i E_i n_i + \frac{g}{2}\int |\phi(x)|^4 dx.$$

However, each metropolis step remains almost the same as in FSS, the only addition is randomization of phases of α_i. Thus combining the approaches preserve cutoff independence with the added benefit of being able to correctly handle systems where interacting BEC mode is different than non-interating BEC.

References

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[2] M. B. Kruk, D. Hryniuk, M. Kristensen, T. Vibel, K. Pawłowski, J. Arlt, and K. Rzążewski, "Microcanonical and canonical fluctuations in atomic Bose-Einstein condensates – Fock state sampling approach", SciPost Phys. **14**, 036 (2023).

[3] M. B. Kruk, T. Vibel, J. Arlt, P. Kulik, K. Pawłowski, and K. Rzążewski, "Fock State Sampling Method – Characteristic temperature of maximal fluctuations for interacting bosons in box potentials", Acta Physica Polonica A (2023).