Fock State Sampling Method for BEC Fluctuations

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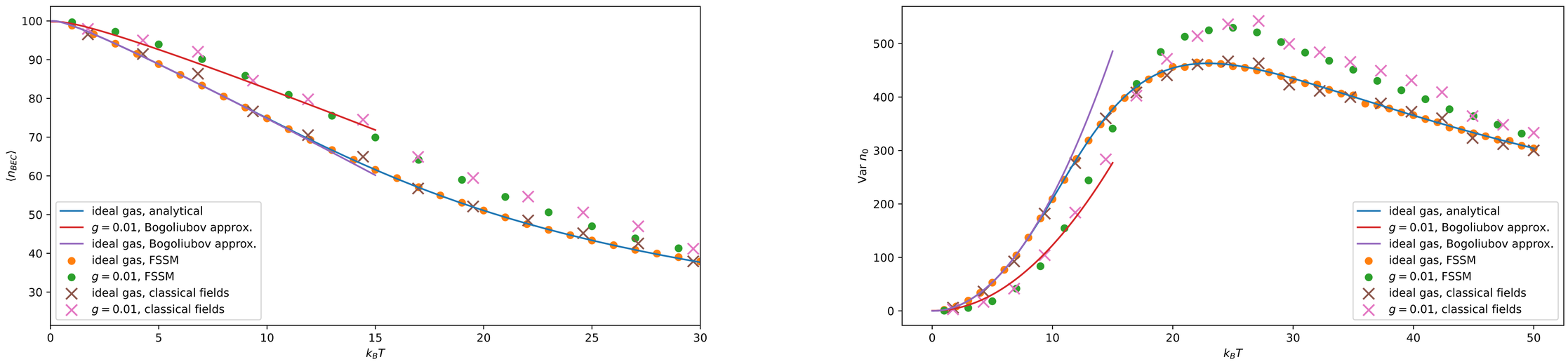

Figure 1: Condensate average occupation and fluctuations in the canonical ensemble, in a 1D box with periodic boundary conditions: comparison of the FSSM to exact (ideal gas) and classical field [1], and Bogoliubov results with interaction $g > 0$. $g = 0.01$ is in natural $\hbar = m = L = 1$ units with box size L and resultant energy units of $\hbar^2/(mL^2)$.

1 The method

Fock State Sampling Method (FSSM) is a new method for calculating BEC fluctuations developed by our group, which was already put to the test in [2]. 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.

To understand how it works, first consider an ideal gas Hamiltonian (harmonic, ring trap, etc.) $\hat{\mathcal{H}}_0$ and a multimode Fock state $|\phi\rangle = |n_0, n_1, n_2, ...\rangle$, with energy E_ϕ and n_i being the number of particles in mode j. All modes are assumed orthogonal.

FSSM can be described shortly by the following:

0 select initial state ϕ,
1 pick a slightly modified candidate ϕ',
2 calculate $\Delta E = E_{\phi'} - E_\phi$,
3 calculate $\alpha = \exp \frac{\Delta E}{kT}$,
4 set $\phi \leftarrow \phi'$ if $\alpha \leqslant r \in [0, 1)$,
5 go to point 1,

where r is a uniform random number. The innovative part in our method is the update rule which determines how we pick the candidate $\phi' = (n_0, n_1, n_2, ...)$. Let $p_A(\phi, i)$ be the probability of moving particle *from* mode i and $p_B(\phi, j)$ be the probability of moving particle *to* mode j. Motivated by the Bose enhancement phenomenon we set

$$p_A(i) \propto n_i, \quad p_B(j) \propto n_j + 1. \tag{1}$$

For the canonical ensemble the total number of particles is fixed, so for every particle we take from one mode we need to put it somewhere else, thus we get the total probability of taking a particle from mode i and putting it in mode j

$$p(\phi, i \to j) = p_A(\phi, i) p_B(\phi, j)$$

for a candidate

$$\phi' = (..., n_i - 1, ..., n_j + 1, ...).$$

The simple product of probabilities implies that the choice of i and j is statistically independent. $p(\phi, i \to j)$ is a proposal distribution in a sense of a Metropolis algorithm. The Bose-enhanced update rule dramatically increases the efficiency of updates for the highly occupied modes while leaving updates in the tails at a physically sensible rate.

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:

$$E = \langle \phi | \hat{\mathcal{H}} | \phi \rangle,$$

where ϕ are the eigenstates of $\hat{\mathcal{H}}_0$, that is

$$\hat{\mathcal{H}}_0 |\phi\rangle = E_\phi |\phi\rangle = (\sum_i E_i n_i) |\phi\rangle.$$

The energy approximation E can be expanded using mode occupation numbers n_i to

$$E = \sum_i E_i n_i + \frac{g}{2} \sum_i h_{ii}(n_i - 1) n_i + 2g \sum_{i<j} h_{ij} n_i n_j.$$

which allows for efficient computation of ΔE once the overlaps h_{ij} have been pre-computed.

2 Weights

Equation (1) paints a good picture of how we want to pick the i, j modes but one can notice that both low and high energy modes have the same probability of being picked, which is wasteful as jumps in higher modes are relatively rare. To remedy this problem, we introduce additional weighting by Boltzmann factors, that is

$$p_A(i) \propto \exp(-\frac{E_i}{T_f}) n_i, \quad p_B(j) \propto \exp(-\frac{E_j}{T_f})(n_j + 1),$$

where T_f is some "fictitious temperature". Physical state functions don't depend on T_f. This modification has additional benefit: we can change in a continuous way the acceptance rate in the Metropolis algorithm (higher T_f decreases acceptance as we will be picking higher modes more often), which boosts the thermalization rate of the algorithm.

3 Interaction quadratic form

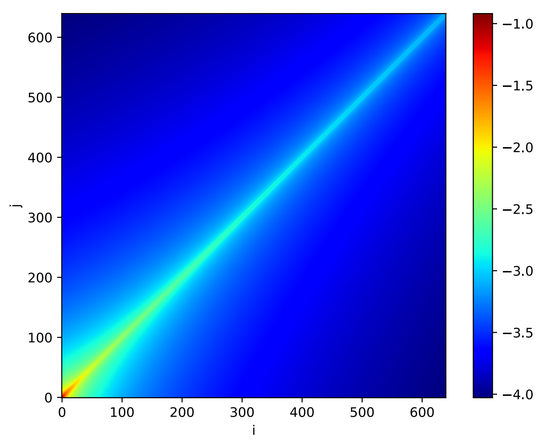

Figure 2: Log plot of h_{ij} matrix for a harmonic trap.

Grouping terms in the expression (2) for the energy gives us

$$E = \sum_i (E_i - \frac{g h_{ii}}{2}) n_i + g \sum_{i,j} \tilde{h}_{ij} n_i n_j,$$

where $\tilde{h}$ is just h with rescaled diagonal by a factor of 2. With periodic boundary conditions $h_{ij} = 0, 1$ and the interaction energy can be computed fast, however for the harmonic potential case, it is not so easy. Naive, brute force computing of the interaction energy is of complexity $O(m^2)$, where m is the number of occupied modes. We need a better approach. Figure 2 illustrates h_{ij} for the harmonic trap case: it is a real, symmetric (but not positive definite!) matrix that we can diagonalize. The idea is to perform "naive" interaction energy calculation but this time, we limit our computations to the "most important" part of the eigenspace. Our preliminary result show that eigensubspace built with about 10^D (D=number of dimensions) eigenvectors is sufficient for accuracy above 99% in calculating the interaction energy.

4 The implementation

The implementation of FSSM consists of the main simulation program and several helper scripts and programs to analyze and plot data. Computation intensive simulation is written in plain C. Parallelisation of our code is trivial: we run multiple independent simulations. Code will be publicly available under a permissive or copyleft license.

(2)

References

[1] M. Kruk, M. Łebek, and K. Rzążewski, "Statistical properties of cold bosons in a ring trap", Phys. Rev. A **101**, 023622 (2020).

[2] M. B. Christensen, T. Vibel, A. J. Hilliard, M. B. Kruk, K. Pawłowski, D. Hryniuk, K. Rzążewski, M. A. Kristensen, and J. J. Arlt, "Observation of microcanonical atom number fluctuations in a bose-einstein condensate", Phys. Rev. Lett. **126**, 153601 (2021).