Exact Numerical Study of Rotating Ideal Bose-Einstein Condensates
Antun Balaž1, Ivana Vidanović1, Axel Pelster ${ }^{2,3}$, Aleksandar Bogojević ${ }^{1}$
${ }^{1}$ Scientific Computing Laboratory, Institute of Physics Belgrade, Pregrevica 118, 11080 Belgrade, Serbia
${ }^{2}$ Fachbereich Physik, Universität Duisburg-Essen, Lotharstrasse 1, 47048 Duisburg, Germany
${ }^{3}$ Universität Potsdam, Campus Golm, Karl-Liebknecht-Strasse 24/25, 14476 Potsdam-Golm, Germany

Motivation: Semiclassical (SC) treatment of ideal Bose-Einstein condensates (BEC) was previously used [1] to describe results of recent ex periments with fast-rotating ${ }^{87} \mathrm{Rb}$ atoms in an anharmonic trap [2]. We apply newly developed abitrary-order short-time propagator expansion technique [3] to exactly calculate static and dynamic properties of such condensates and to estimate the quality of SC results. We also show that first correction to SC result for $T$ diverges for critical rotation where only the presented exact approach can be used to assess SC results.

## Properties of ideal BECs

- Grand-canonical ensemble
$\star$ Cumulant expansion for the free energy

$$
\mathcal{F}=-\frac{1}{\beta} \ln \mathcal{Z}=\frac{1}{\beta} \sum_{k} \ln \left(1-e^{-\beta\left(E_{k}-\mu\right)}\right)=-\frac{1}{\beta} \sum_{m=1}^{\infty} \frac{e^{m \beta \mu}}{m} \mathcal{Z}_{1}(m \beta)
$$

where $\mathcal{Z}_{1}(m \beta)$ is one-particle partition function
$\star$ Total number of particles is sum of the ground-state occupancy $N_{0}$ and the number of thermal particles, given by $-\partial \mathcal{F} / \partial \mu$
$\star$ In BEC phase we set $\mu=E_{0}$, while in the gas phase $N_{0}=0$

- Static properties
$\star$ The condensation temperature $T_{\mathrm{c}}$ is defined by $\mu=E_{0}$ and $N_{0}=0$, where:

$$
N_{0}=N+\partial \mathcal{F} / \partial \mu=N-\sum_{m=1}^{\infty}\left(e^{m \beta \mu} \mathcal{Z}_{1}(m \beta)-1\right)
$$

$\star$ This also determines the condensate fraction $N_{0} / N$ for $T<T_{\mathrm{c}}$
$\star$ Diagonal density matrix elements $\left\langle\hat{\Psi}^{\dagger}(\vec{r}) \hat{\Psi}(\vec{r})\right\rangle$ give the density profile

$$
n(\vec{r})=N_{0}\left|\psi_{0}(\vec{r})\right|^{2}+\sum_{n \geq 1} N_{n}\left|\psi_{n}(\vec{r})\right|^{2}
$$

where thermal occupancies $N_{n}$ are given by the Bose-Einstein distribution

- Dynamic properties
* Time-of-flight absorption pictures are obtained by switching off the trapping potential and allowing the gas to freely expand
* The density profile after time $t$ is given by

$$
n(\vec{r}, t)=N_{0}\left|\psi_{0}(\vec{r}, t)\right|^{2}+\sum_{n \geq 1} N_{n}\left|\psi_{n}(\vec{r}, t)\right|^{2}
$$

where $\psi_{n}(\vec{r}, t)=\frac{1}{(2 \pi)^{3}} \int \mathrm{~d}^{3} \vec{k} \mathrm{~d}^{3} \vec{R} e^{-i \omega_{k} t+i \vec{k} \cdot \vec{r}-i \vec{k} \cdot \vec{R}} \psi_{n}(\vec{R})$

## - SC approximation

*Static and some dynamic properties of BECs can be calculated in SC approach [1]
*First correction to SC result for $T_{c}$ is known for harmonic [3] trap and can be calculated also for other trapping potentials

* However, for critically rotating ideal BEC in a quartic anharmonic trap $V_{\text {BEC }}[1,2]$, first correction

$$
\frac{\Delta T_{\mathrm{c}}}{T_{\mathrm{c}}^{0}}=-\frac{2 \zeta(3 / 2) E_{0}}{5 \zeta^{3 / 5}(5 / 2)}\left(\frac{M^{2} \pi}{4 k \hbar^{6} \omega_{z}^{2}}\right)^{1 / 5} \frac{1}{N^{2 / 5}}
$$

diverges for small anharmonicity $k$ and cannot be used to assess SC result

## Arbitrary-order short-time propagator expansion

- Discretized effective potential
$\star$ Recently developed approach [4] allows analytic calculation of the arbitrary-order short-time expansion of the non-relativistic many-body propagator, expressed in terms of the discretized effective potential $W$ :

$$
A(a, b ; \epsilon)=\frac{1}{(2 \pi \epsilon)^{M d / 2}} \exp \left\{-\frac{(b-a)^{2}}{2 \epsilon}-\epsilon W\left(\frac{a+b}{2}, \frac{b-a}{2} ; \epsilon\right)\right\}
$$

where $M$ is the number of particles in $d$ spatial dimensions
$\star$ The expansion of the effective potential up to order $\epsilon^{p-1}$ yields propagato values correct to order $\epsilon^{p}$

- Calculation of one-particle eigenvalues and eigenstate $\star$ Approach based on the exact numerical diagonalization of the spacediscretized evolution operator matrix $[5,6]$

$$
A_{n m}(\epsilon, \Delta)=\langle n \Delta| e^{-\epsilon \tilde{H}}|m \Delta\rangle \cdot \Delta
$$

$\star$ Eigenvectors of matrix $A_{n m}$ are space-discretized eigenvectors of the Hamiltonian $\hat{H}$, while eigenvalues are $e^{-\epsilon E_{n}}$

Numerical results: Static properties of BECs

- Calculation of energy eigenvalues and $T$


Errors of numerically calculated $E_{0}$ vs. diagonalization
parameter $\epsilon$ for critical rotation $\Omega / \omega_{\perp}=1$

- Condensate fraction



effective action, with $T_{c}^{0}=110 \mathrm{nK}$
 Number of particles vs. $T_{\mathrm{c}}[\mathrm{KK}]$ for different rotation
frequencies, obtained with $p=18$ effective action


Comparison of $N_{0} / N$ vs. $T$ for critical rotation, obapproach, for several values of $k / k_{\text {exp }}$.

```
Experimental setup: Fast-rotating BEC
```

$\star$ Paris group of J. Dalibard recently realized critically rotating BEC of $3 \cdot 10^{5}$ atoms of ${ }^{87} \mathrm{Rb}$ in an axially symmetric trap [2]
*The small quartic anharmonicity in $x-y$ plane was used to keep the condensate trapped even at the critical rotation frequency
$\star$ Effective trapping potential: $V_{\text {BEC }}=\frac{1}{2} M\left(\omega_{\perp}^{2}-\Omega^{2}\right) r_{\perp}^{2}+\frac{1}{2} M \omega_{z}^{2} z^{2}+\frac{k_{\text {exp }}}{4} r_{\perp}^{4}$ where $\omega_{\perp}=2 \pi \times 64.8 \mathrm{~Hz}, \omega_{z}=2 \pi \times 11.0 \mathrm{~Hz}, k_{\exp }=2.6 \times 10^{-11} \mathrm{Jm}^{4}$

Numerical results: Dynamic properties of BECs

- Critical rotation: Time-of-flight absorption graphs at $T=10 \mathrm{nK}$, obtained with $p=21$ effective action. Linear profile size is $54 \mu \mathrm{~m}$.

- Overcritical rotation: Time-of-flight graphs for $\Omega / \omega_{\perp}=1.05$ at $T=10$ nK , obtained with $p=21$ effective action. Linear profile size is $54 \mu \mathrm{~m}$.



## Summary and outlook

$\star$ Exact numerical treatment used to asses quality of SC approximation $\star$ SC results have accuracy of 1-3\% in the considered range of parameters $\star$ Numerical approach necessary to assess SC results near the critical rotation $\star$ Formation and evolution of vortices requires interactions to be introduced

## References

1] S. Kling, A. Pelster, PRA 76, 023609 (2007)
2] V. Bretin, S. Stock, Y. Seurin, J. Dalibard, PRL 92, 050403 (2004) [3] S. Grossmann, M. Holthaus, PLA 208, 188 (1995)
[4] A. Balaž, A. Bogojević, I. Vidanović, A. Pelster, PRE 79, 036701 (2009) [5] A. Sethia, S. Sanyal, Y. Singh, J. Chem. Phys. 93, 7268 (1990) [6] I. Vidanović, A. Bogojević, A. Balaž, A. Belić, submitted to PRE Support: Serbian Ministry of Science, German Academic Exchange Ser vice (DAAD), and European Commission through research projects PI-BEC, OI141035, CX-CMCS, EGEE-III, and SEE-GRID-SCI

## DAAD



EGCe

