Ultra-fast Converging Path Integral Approach for Rotating Ideal Bose Gases*

A. Balaž[1], I. Vidanović[1], A. Bogojević[1], A. Pelster[2,3]

[1]Scientific Computing Laboratory, Institute of Physics Belgrade
Pregrevica 118, 11080 Belgrade, Serbia
http://www.scl.rs/

[2]Fachbereich Physik, Universität Duisburg-Essen
Lotharstrasse 1, 47048 Duisburg, Germany

[3]Institut für Theoretische Physik, Freie Universität Berlin
Arnimalee 14, 14195 Berlin, Germany

*Supported by the Serbian-German bilateral research project PI-BEC, Serbian Ministry of Science research project OI141035, and EU CX-CMCS Centre of Excellence grant.

Overview

- Effective actions for path integrals
  - Numerical approach to path integrals
  - Discretized effective actions
  - Effective actions for many-body systems
- Rotating ideal BECs
  - Energy eigenvalues and eigenstates
  - Calculation of global properties of BECs
  - Calculation of density profiles of BECs
  - Time-of-flight graphs for BECs
- Numerical results
  - Energy eigenvalues and eigenstates
  - Global properties of BECs
  - Density profiles of BECs
  - Time-of-flight graphs for BECs
- Concluding remarks

Path integral formalism

- Continual amplitude $A(\alpha,\beta;T)$ is obtained in the limit $N\to\infty$ of the discretized amplitude $A_N(\alpha,\beta;T)$,

$$A(\alpha,\beta;T)=\lim_{N\to\infty}A_N(\alpha,\beta;T)$$

- Discretized amplitude A_N is expressed as a multiple integral of the function e^{-S_N}, where S_N is called discretized action
- For a theory defined by the Lagrangian $L=\frac{1}{2}\,\dot{q}^2+V(q)$, (naive) discretized action is given by

$$S_N=\sum_{n=0}^{N-1}\left(\frac{\delta_n^2}{2\epsilon}+\epsilon V(\bar{q}_n)\right)\,,$$

where $\delta_n=q_{n+1}-q_n$, $\bar{q}_n=\frac{q_{n+1}+q_n}{2}$.

Discretized effective actions

- Discretized actions can be classified according to the speed of convergence of discretized path integrals to continuum
- It is possible to introduce different discretized actions which contain additional terms compared to the naive action, substantially speeding up the convergence
- We have derived, in a systematic way, an approach for obtaining higher level discretized effective actions for general non-relativistic many body systems
- Discretized effective actions of level p lead to $1/N^p$ convergence of discretized amplitudes to the continuum

Effective actions for many-body systems

- We start from Schrödinger's equation for the amplitude $A(q, q'; \epsilon)$ for a system of M non-relativistic particles in d spatial dimensions

$$\left[\frac{\partial}{\partial\epsilon} - \frac{1}{2}\sum_{i=1}^{M}\triangle_i + V(q)\right] A(q, q'; \epsilon) = 0$$

$$\left[\frac{\partial}{\partial\epsilon} - \frac{1}{2}\sum_{i=1}^{M}\triangle'_i + V(q')\right] A(q, q'; \epsilon) = 0$$

- Here $\triangle_i$ and $\triangle'_i$ are d-dimensional Laplacians over initial and final coordinates of the particle i, while q and q' are $d \times M$ dimensional vectors representing positions of all particles at the initial and final time.

Equation for the ideal effective potential

- If we express short-time amplitude $A(q,q';\epsilon)$ by the ideal discretized effective potential W

$$A(q,q';\epsilon)=\frac{1}{(2\pi\epsilon)^{dM/2}}\exp\left[-\frac{\delta^2}{2\epsilon}-\epsilon W\right]$$

we obtain equation for the effective potential in terms of $x=\delta/2$, $\bar{x}=(q+q')/2$, $V_\pm=V(\bar{x}\pm x)$

$$W+x\cdot\partial\,W+\epsilon\frac{\partial W}{\partial\epsilon}-\frac{1}{8}\,\epsilon\bar{\partial}^2W-\frac{1}{8}\,\epsilon\partial^2W+\frac{1}{8}\,\epsilon^2(\bar{\partial}W)^2+ \\ +\frac{1}{8}\,\epsilon^2(\partial W)^2=\frac{V_++V_-}{2}$$

Recursive relations

- As before, the effective potential is given as a series

$$W(x,\bar{x};\epsilon)=\sum_{m=0}^{\infty}\sum_{k=0}^{m}W_{m,k}(x,\bar{x})\,\epsilon^{m-k}$$

where

$$W_{m,k}(x,\bar{x})=x_{i_1}x_{i_2}\cdots x_{i_{2k}}c_{m,k}^{i_1,\ldots,i_{2k}}(\bar{x})$$

- Coefficients $W_{m,k}$ are obtained from recursive relations

$$\begin{aligned}8\,(m+k+1)\,W_{m,k}&=\bar{\partial}^2W_{m-1,k}+\partial^2W_{m,k+1}-\\&-\sum_{l=0}^{m-2}\sum_{r}(\bar{\partial}W_{l,r})\cdot(\bar{\partial}W_{m-l-2,k-r})-\\&-\sum_{l=1}^{m-2}\sum_{r}(\partial W_{l,r})\cdot(\partial W_{m-l-1,k-r+1})\end{aligned}$$

Rotating ideal Bose gases (1)

- Weakly-interacting dilute gases
- Bose-Einstein condensates usually realized in harmonic magneto-optical traps
- Fast-rotating Bose-Einstein condensates - one of the hallmarks of a superfluid is its response to rotation
- Paris group (J. Dalibard) has recently realized critically rotating BEC of $3 \cdot 10^5$ atoms of ^{87}Rb in an axially symmetric trap - we model this experiment
- The small quartic anharmonicity in $x - y$ plane was used to keep the condensate trapped even at the critical rotation frequency [PRL **92**, 050403 (2004)]

Rotating ideal Bose gases (2)

- We apply the developed discretized effective approach to the study of properties of such (fast-rotating) Bose-Einstein condensates
- We calculate large number of energy eigenvalues and eigenvectors of one-particle states
- We numerically study global properties of the condensate
  - T_c as a function of rotation frequency Ω
  - ground state occupancy N_0/N as a function of temperature
- We calculate density profiles of the condensate and time-of-flight absorption graphs
- $V_{BEC} = \frac{M}{2}(\omega_\perp^2 - \Omega^2) r_\perp^2 + \frac{M}{2}\omega_z^2 z^2 + \frac{k}{4} r_\perp^4$, $\omega_\perp = 2\pi \times 64.8$ Hz, $\omega_z = 2\pi \times 11.0$ Hz, $k = 2.6 \times 10^{-11}$ Jm^{-4}

Rotating ideal Bose gases (3)

- Within the grand-canonical ensemble, the partition function of the ideal Bose gas is

$$\mathcal{Z} = \sum_\nu e^{-\beta(E_\nu - \mu N_\nu)} = \prod_k \frac{1}{1 - e^{-\beta(E_k-\mu)}}$$

The free energy is given by

$$\mathcal{F} = -\frac{1}{\beta}\ln \mathcal{Z} = \frac{1}{\beta}\sum_k \ln(1-e^{-\beta(E_k-\mu)}) = -\frac{1}{\beta}\sum_{m=1}^{\infty}\frac{e^{m\beta\mu}}{m}\mathcal{Z}_1(m\beta)$$

where $\mathcal{Z}_1(m\beta)$ is a single-particle partition function

- The number of particles is given as

$$N = -\frac{\partial \mathcal{F}}{\partial \mu} = \sum_{m=1}^{\infty}(e^{m\beta\mu}\mathcal{Z}_1(m\beta) - 1)$$

Rotating ideal Bose gases (4)

- The usual approach to BEC is to treat the ground state separately, and fix μ below the condensation temperature $\mu = E_0$
- Below the condensation temperature we have

$$N = N_0 + \sum_{m=1}^{\infty} (e^{m\beta E_0} \mathcal{Z}_1(m\beta) - 1)$$

- The condensation temperature T_c is thus defined by the condition:

$$\frac{N_0}{N} = 1 - \frac{1}{N} \sum_{m=1}^{\infty} (e^{m\beta_c E_0} \mathcal{Z}_1(m\beta_c) - 1) = 0$$

Energy eigenvalues and eigenstates

- Single-particle eigenvalues and eigenstates are sufficient for the calculation of BEC condensation temperature
- The most efficient approach for low-dimensional systems is direct diagonalization of space-discretized propagator $e^{-\epsilon\hat{H}}$, where ϵ is appropriately chosen artificial short-time of propagation (no time-slices approximation)
- On a given space grid, matrix elements of the propagator are just short-time aplitudes
- If ϵ is chosen so that $\epsilon < 1$, such amplitudes can be directly (analytically) calculated using previously derived effective actions with the high convergence level p
- The obtained eigenvalues are $e^{-\epsilon E_n}$, and the obtained eigenvectors are space-discretized eigenvectors ψ_n

Details on the calculation of global properties of BECs

- E_n can be obtained by the direct diagonalization of the space-discretized propagator, and single-particle partition functions $\mathcal{Z}_1(m\beta)$ can be the calculated as

$$\mathcal{Z}_1(m\beta) = \sum_n e^{-m\beta E_n}$$

- This is suitable for low temperatures, when higher energy levels (not accessible in the diagonalziation) are negligibe
- For mid-range temperatures, $\mathcal{Z}_1$ can be numerically calculated as a sum of diagonal amplitudes, and then E_0 may be extracted from the free energy

Density profiles of Bose-Einstein condensates (1)

- Density profile is given in terms of the two-point propagator $\rho(\vec{r}_1, \vec{r}_2) = \langle \hat{\Psi}^\dagger(\vec{r}_1)\hat{\Psi}(\vec{r}_2)\rangle$ as a diagonal element, $n(\vec{r}) = \rho(\vec{r}, \vec{r})$
- For the ideal Bose gas, the density profile can be written as

$$n(\vec{r}) = N_0|\psi_0(\vec{r})|^2 + \sum_{n\geq 1} N_n|\psi_n(\vec{r})|^2$$

  where the second term represents thermal density profile
- Vectors ψ_n represent single-particle eigenstates, while occupancies N_n are given by the Bose-Einstein distribution for $n \geq 1$,

$$N_n = \frac{1}{e^{\beta(E_n - E_0)} - 1}$$

Density profiles of Bose-Einstein condensates (2)

- Using the cumulant expansion of occupancies and spectral decomposition of amplitudes, the density profile can be also written as

$$n(\vec{r}) = N_0|\psi_0(\vec{r})|^2 + \sum_{m\geq 1}\left[e^{m\beta E_0}A(\vec{r},0;\vec{r},m\beta\hbar) - |\psi_0(\vec{r})|^2\right]$$

  where $A(\vec{r},0;\vec{r},m\beta\hbar)$ represents the (imaginary-time) amplitude for one-particle transition from the position $\vec{r}$ in $t=0$ to the position $\vec{r}$ in $t=m\beta\hbar$
- Both definitions are mathematically equivalent
- The first one is more suitable for low temperatures, while the second one is suitable for mid-range temperatures

Time-of-flight graphs for BECs (1)

- In typical BEC experiments, a trapping potential is switched off and gas is allowed to expand freely during a short time of flight t (of the order of 10s of ms)
- The absorption picture is then taken, and it maps the density profile to the plane perpendicular to the laser beam
- For the ideal Bose condensate, the density profile after time t is given by

$$n(\vec{r},t) = N_0|\psi_0(\vec{r},t)|^2 + \sum_{n\geq 1} N_n|\psi_n(\vec{r},t)|^2$$

where

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

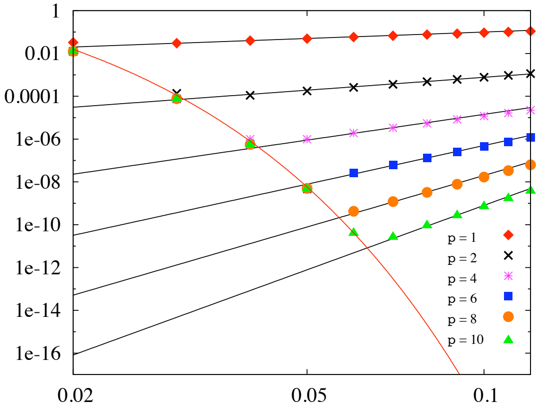
Time-of-flight graphs for BECs (2)

- For mid-range temperatures we can use mathematically equivalent definition of the density profile

$$n(\vec{r},t) = N_0|\psi_0(\vec{r},t)|^2 + \sum_{m\geq 1}\left[e^{m\beta E_0}\int \frac{\mathrm{d}^3\vec{k}_1\,\mathrm{d}^3\vec{k}_2\,\mathrm{d}^3\vec{R}_1\,\mathrm{d}^3\vec{R}_2}{(2\pi)^6}\times\right.$$
$$\left. e^{-i(\omega_{\vec{k}_1}-\omega_{\vec{k}_2})t+i(\vec{k}_1-\vec{k}_2)\cdot\vec{r}-i\vec{k}_1\cdot\vec{R}_1+i\vec{k}_2\cdot\vec{R}_2}\,A(\vec{R}_1,0;\vec{R}_2,m\beta\hbar) - |\psi_0(\vec{r},t)|^2\right]$$

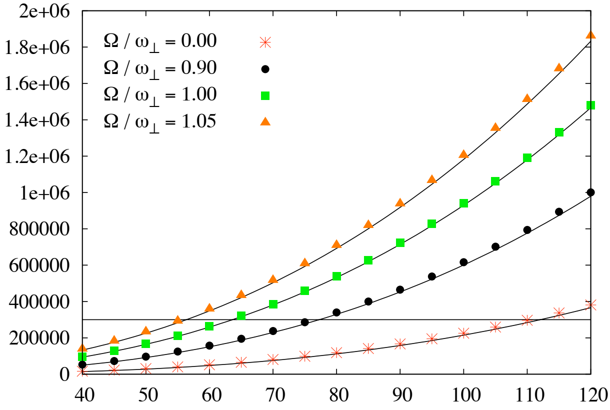
- In both approaches it is first necessary to calculate E_0 and $\psi_0(\vec{r})$ using direct diagonalization or some other method
- FFT is ideally suitable for numerical calculations of time-of-flight graphs

Energy eigenvalues and eigenstates



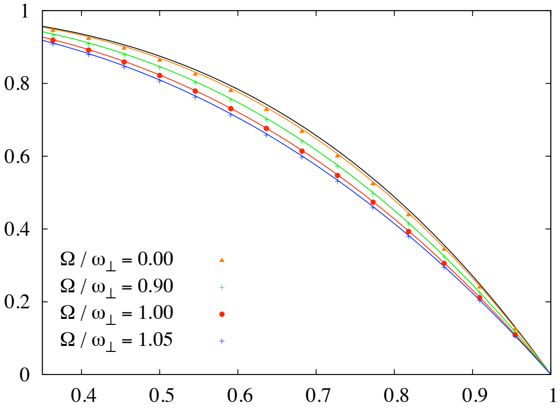
Deviations from the exact ground-state energy vs. ϵ for V_{BEC} (critical rotation). The error is proportional to ϵ^p. The red curve is the discretization error (analytically known).

Calculation of the condensation temperature



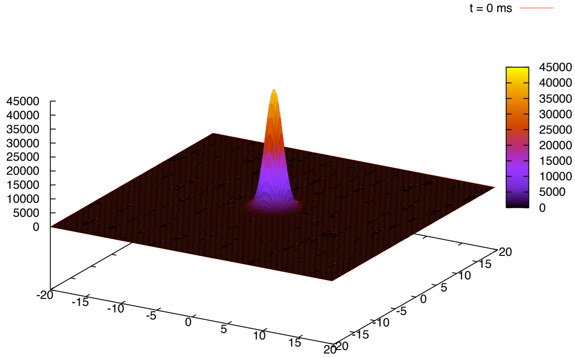
Number of particles as a function of T_c [nK] for different rotation frequencies, obtained with $p = 18$ effective action.

Calculation of the ground-state occupancy



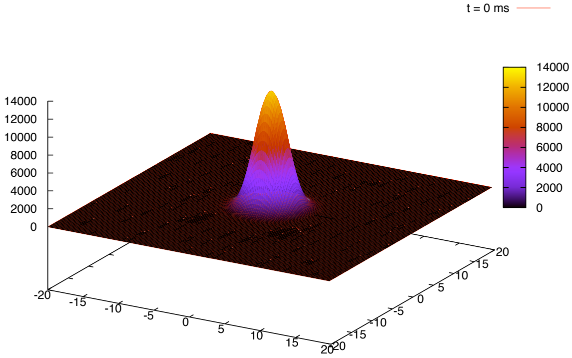
Ground-state occupancy N_0/N as a function of T/T_c^0 for different rotation frequencies, obtained with $p = 18$ effective action ($T_c^0 = 110$ nK used as a typical scale in all cases).

Density profiles of Bose-Einstein condensates (1)



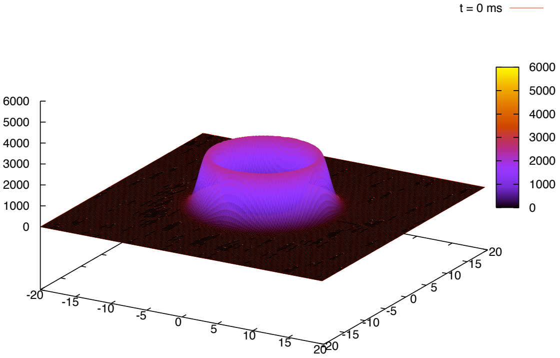
Density profile in $x - y$ plane for the condensate at under-critical rotation $\Omega/\omega_\perp = 0.9$, $T = 10$ nK $< T_c = 76.8$ nK. The linear size of the profile is 54 μm.

Density profiles of Bose-Einstein condensates (2)



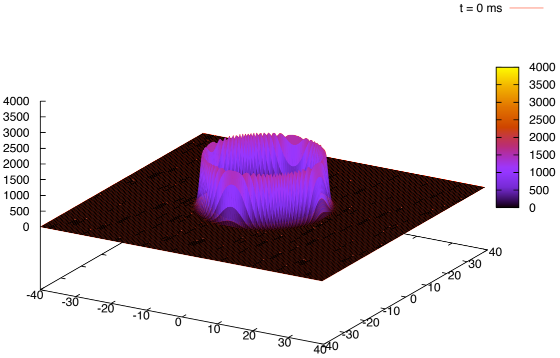
Density profile in $x - y$ plane for the condensate at critical rotation $\Omega/\omega_\perp = 1$, $T = 10$ nK $< T_c = 63.3$ nK. The linear size of the profile is 54 μm.

Density profiles of Bose-Einstein condensates (3)



Density profile in $x-y$ plane for the condensate at over-critical rotation $\Omega/\omega_\perp = 1.05$, $T = 10$ nK $< T_c = 55.3$ nK. The linear size of the profile is 54 μm.

Density profiles of Bose-Einstein condensates (4)



Density profile in $x - y$ plane for the condensate at over-critical rotation $\Omega/\omega_\perp = 1.2$, $T = 10$ nK $< T_c = 49.1$ nK. The linear size of the profile is 108 μm.

Time-of-flight graphs for BECs (1)

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Evolution of the $x - y$ density profile with the time-of-flight for the condensate at under-critical rotation $\Omega/\omega_\perp = 0.9$, $T = 10$ nK $< T_c = 76.8$ nK. The linear size of the profile is 54 μm.

Time-of-flight graphs for BECs (2)

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Evolution of the $x - y$ density profile with the time-of-flight for the condensate at critical rotation $\Omega/\omega_{\perp} = 1$, $T = 10$ nK $< T_c = 63.3$ nK. The linear size of the profile is 54 μm.

Time-of-flight graphs for BECs (3)

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Evolution of the $x - y$ density profile with the time-of-flight for the condensate at over-critical rotation $\Omega/\omega_\perp = 1.05$, $T = 10$ nK $< T_c = 55.3$ nK. The linear size of the profile is 54 μm.

Time-of-flight graphs for BECs (4)

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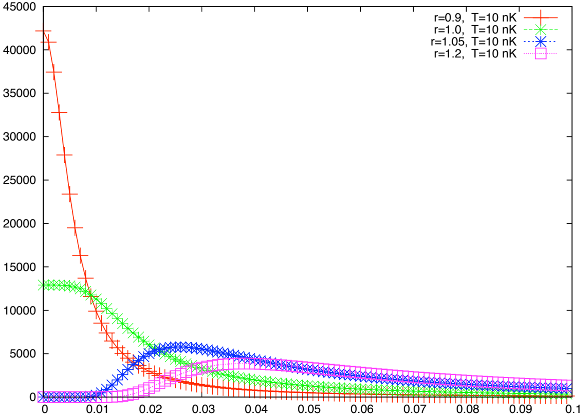
Evolution of the $x-y$ density profile with the time-of-flight for the condensate at over-critical rotation $\Omega/\omega_\perp = 1.2$, $T = 10$ nK $< T_c = 49.1$ nK. The linear size of the profile is 108 μm.

Time evolution of the density at the origin



Time evolution [s] of the condensate density at the origin of $x - y$ plane for the condensate at various rotation frequencies $(r = \Omega/\omega_\perp)$ for $T = 10$ nK $< T_c$.

Conclusions

- A new method for numerical calculation of path integrals applied to the study of ideal Bose gases
- High-order discretized effective actions used for efficient numerical calculation of global and local properties of fast-rotating BECs
  - Single-particle eigenvalues and eigenstates
  - Condensation temperature and ground-state occupancy
  - Density profiles
  - Time-of-flight graphs
- Overcritical rotation substantially increases time scale for free expansion after trapping potential is switched off

Further applications

- Ground states of low-dimensional quantum systems
- Properties of interacting BECs
  - Gross-Pitaevskii equation
  - Effective actions for time-dependent potentials
- Properties of rotating Fermionic gases
- Related applications: Quantum gases with disorder (Anderson localization)

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