Ultra-fast Converging Path Integral Approach for Ideal Bose Gases

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Overview

- Introduction
  - General properties of path integrals
  - Formulation of the path integral formalism
  - Monte Carlo numerical approach
  - Discretized effective actions
- Effective actions
  - Gaussian halving: one-particle systems in $d = 1$
  - Euler's summation formula for path integrals
  - Recursive approach: many-body systems
  - Diagrammatic representation of effective actions
- Ideal Bose gases
  - Energy eigenvalues and eigenstates
  - Calculation of global properties of BECs
  - Density profiles of BECs
  - Time-of-flight graphs for BECs
- Concluding remarks

General properties of path integrals

- Basic ideas on path integral formalism can be found in: P. A. M. Dirac, Physikalische Zeitschrift der Sowietunion **3**, 64 (1933) - Lagrangian formulation of quantum mechanics
- Richard Feynman developed the formalism we use today [R. P. Feynman, Rev. Mod. Phys. **20**, 367 (1948)]
- Contrary to the classical physics, where (usually) there is only one trajectory of the system for a given set of initial (boundary) conditions, in path integral formalism of the quantum theory we have to take into account all possible evolutions
- Each of possible trajectories contributes to the transition amplitude through the additive factor $\exp(\frac{i}{\hbar}S)$, where $S = \int L dt$ is the action corresponding to the given trajectory

Formulation of the path integral formalism (1)

- Path integrals originally introduced in quantum mechanics, where the amplitude for transition from some initial state $|\alpha\rangle$ to some final state $|\beta\rangle$ during a time interval T can be written as
$$A(\alpha, \beta; T) = \langle \beta | e^{-\frac{i}{\hbar}\hat{H}T} | \alpha \rangle$$
- The same approach can be used in statistical physics, where partition function Z can be written in a similar fashion
- Path integrals in statistical physics / condensed matter are usually called imaginary-time path integrals, since they can be formally obtained from quantum-mechanical expressions through the formal replacement
$$\frac{i}{\hbar}T \to \beta_t = \frac{1}{k_B T_t}$$
where T_t is the (thermodynamic) temperature of the system

Formulation of the path integral formalism (2)

- For technical reasons, usually we use imaginary time even in quantum mechanical problems ($\frac{i}{\hbar}T \to -\frac{1}{\hbar}T$)
- The standard derivation of the formalism starts from the identity

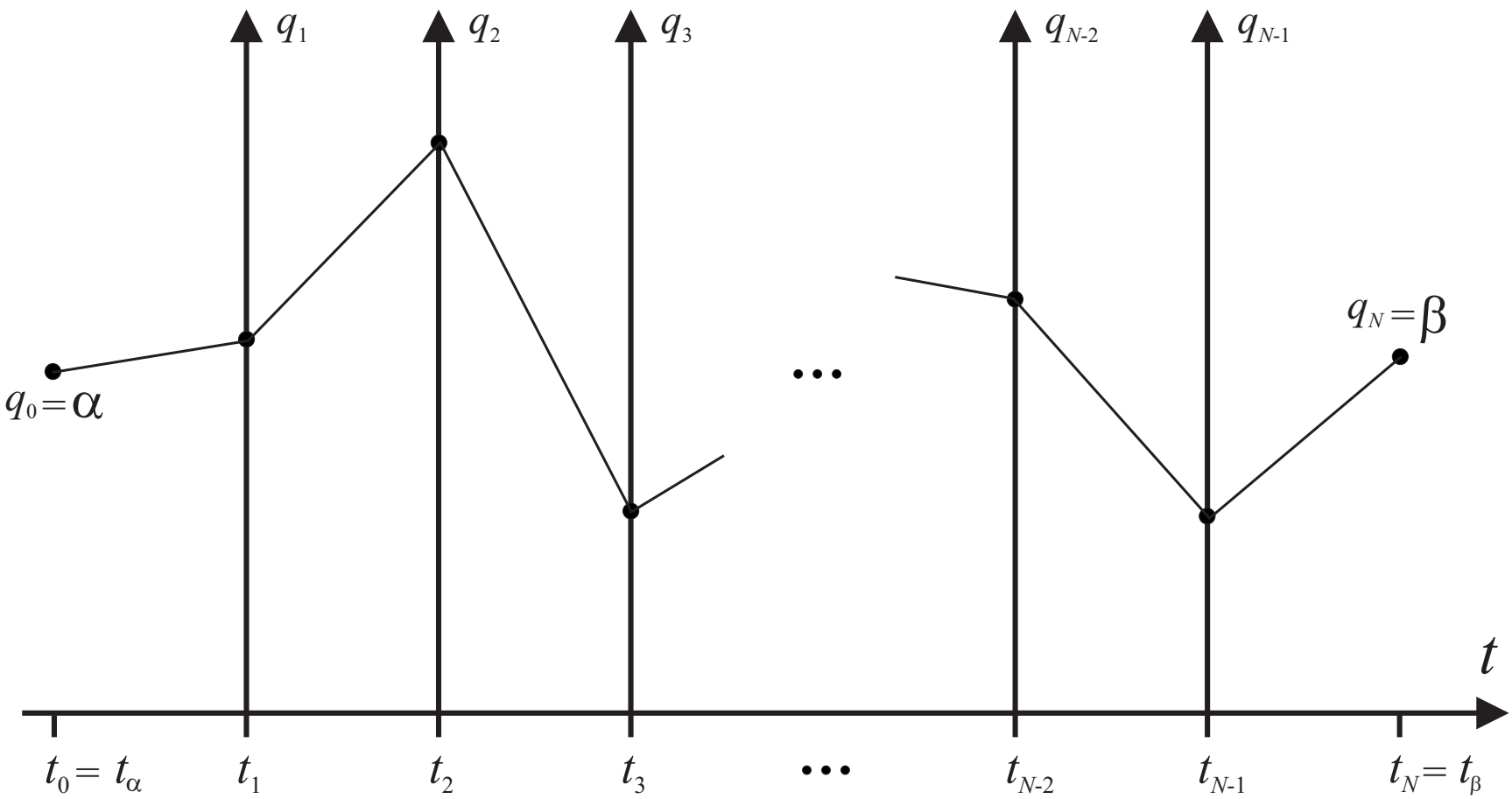
$$A(\alpha,\beta;T) = \int dq_1 \cdots dq_{N-1} A(\alpha,q_1;\epsilon)\cdots A(q_{N-1},\beta;\epsilon)\,,$$

which is obtained by dividing the evolution into N steps of the lenght $\epsilon = T/N$, and by insertion of $N-1$ resolutions of the identity operator between short-time evolution operators. This expression is exact.

- Next step is approximate calculation of short-time amplitudes up to the first order in ϵ, and we get ($\hbar = 1$)

$$A_N(\alpha,\beta;T) = \frac{1}{(2\pi\epsilon)^{N/2}} \int dq_1 \cdots dq_{N-1}\, e^{-S_N}$$

Illustration of the discretization of trajectories



Formulation of the path integral formalism (3)

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

Monte Carlo method

- Monte Carlo (MC) can be defined as a method for solving mathematical problems by using (pseudo-)random numbers
- If implemented properly, MC is guaranteed to converge to the exact value being calculated
- MC allows estimation of errors for calculated quantities, with clear statistical interpretation
- Calculation of integrals is the most common mathematical problem solved using MC method

$$I = \int_\alpha^\beta f(x)\,dx = \int_\alpha^\beta \frac{f(x)}{p(x)} p(x)\,dx = \left\langle \frac{f}{p} \right\rangle_p ,$$

where p is some given probability distribution function,

$$p \geq 0\,, \quad \int_\alpha^\beta p(x)\,dx = 1$$

Numerical approach to the calculation of path integrals (1)

- Path integral formalism is ideally suited for numerical approach, with physical quantities defined by discretized expressions as multiple integrals of the form

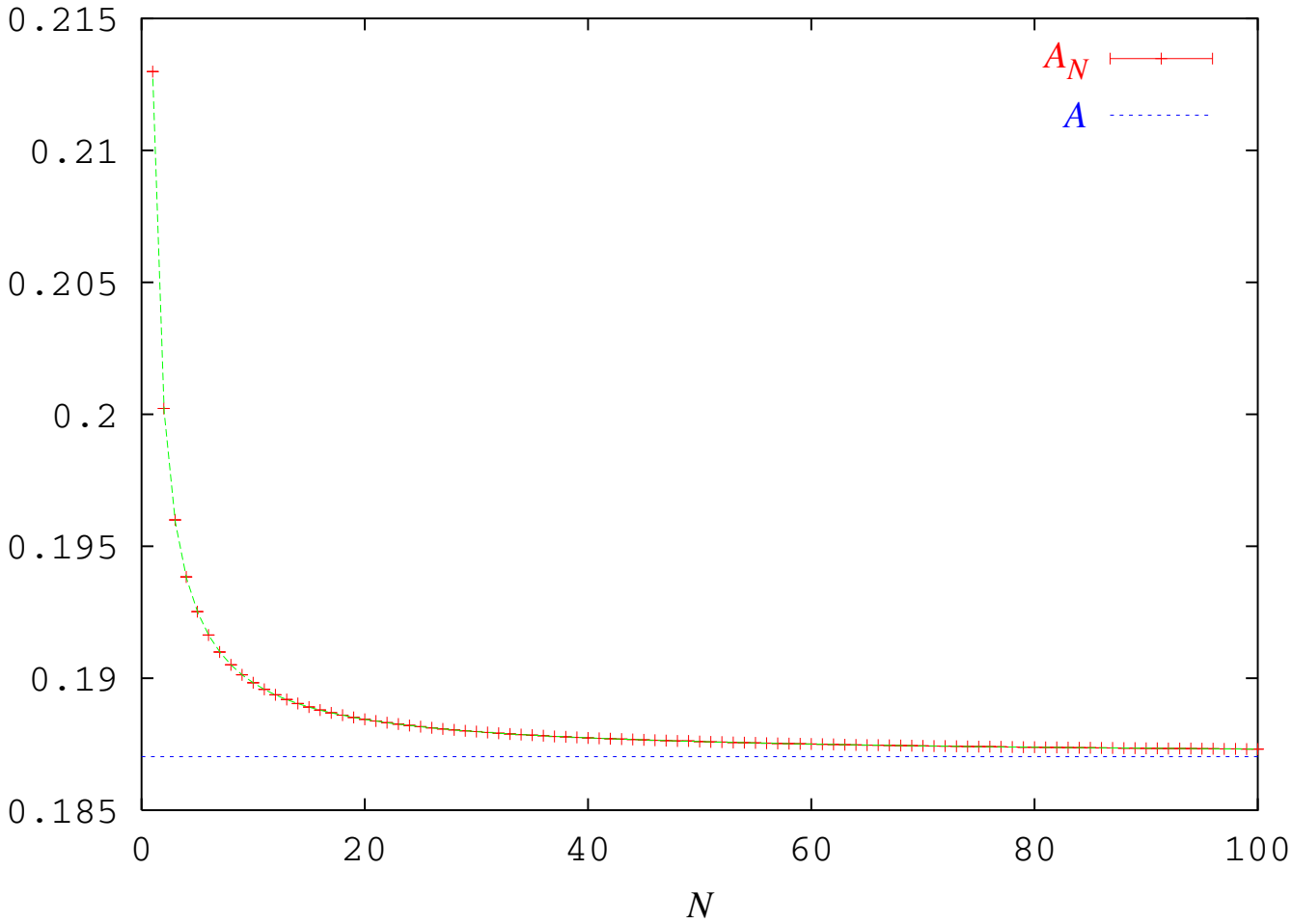
$$\int dq_1 \cdots dq_{N-1}\, e^{-S_N}$$

- Monte Carlo (MC) is the method of choice for calculation of such intergals
- However, although multiple integrals can be calculated very accurately and efficiently by MC, there still remains the difficult $N \to \infty$ limit
- This is what makes the outlined constructive definition of path integrals difficult to use in practical applications

Numerical approach to the calculation of path integrals (2)

- Discretization used in the definition of path integrals is not unique; in fact, the choice of the discretization is of *essential* importance
- Naive discretized action (in the mid-point prescription) gives discretized amplitudes converging to the continuum as slow as $1/N$
- Using special tricks we can get better convergence (e.g. left prescription gives $1/N^2$ convergence when partition function is calculated)
- However, this cannot be done in a systematic way, nor it can be used in all cases (e.g. left prescription cannot be used for systems with ordering ambiguities)

Typical $1/N$ convergence of naively discretized path integrals



Discretized effective actions (1)

- Discretized actions can be classified according to the speed of convergence of discretized path integrals to continuum values
- It is possible to introduce different discretized actions which contain some additional terms compared to the naive discretized action
- These additional terms must vanish in the $N \to \infty$ limit, and should not change continuum values of amplitudes, e.g.

$$\sum_{n=0}^{N-1} \epsilon^3 V'(\bar{q}_n) \to \epsilon^2 \int_0^T dt\, V'(q(t)) \to 0$$

- Additional terms in discretized actions are chosen so that they speed up the convergence of path integrals

Discretized effective actions (2)

- Improved discretized actions have been earlier constructed through several approaches, including
  - generalizations of the Trotter-Suzuki formula
  - improvements in the short-time propagation
  - expansion of the propagator by the number of derivatives
- This improved the convergence of general path integrals for partition functions from $1/N$ to $1/N^4$
- Li-Broughton effective potential

$$V^{LB} = V + \frac{1}{24}\epsilon^2 V'^2 .$$

  in the left prescription gives $1/N^4$ convergence
- Derivation of the above expression from the generalized Trotter formula makes use of the cyclic property of the trace, hence $1/N^4$ convergence is obtained for partition functions only

Improving effective actions

- We present here an approach enabling a substantial speedup in the convergence of path integrals through studying the connection between different discretizations of the same theory
- Using this approach we have derived the integral equation connecting discretized effective actions of different coarseness, which allows their systematic derivation. This leads to improved $1/N^p$ convergence of path integrals for one-particle systems in $d = 1$ - Gaussian halving
- We also present the generalization of this method to many-body systems, based on solving the recursive relations for discretized effective action, which are derived from Schrödinger equation for short-time amplitudes - recursive approach

Ideal discretization (1)

- Ideal discretized action S^* is defined as the action giving exact continual amplitudes $A_N = A$ for any discretization N
- For the free particle, the naive discretized action is ideal
- From the completeness relation

$$A(\alpha, \beta; T) = \int dq_1 \cdots dq_{N-1}\, A(\alpha, q_1; \epsilon) \cdots A(q_{N-1}, \beta; \epsilon)\,,$$

it follows that the ideal discretized action S_n^* for the propagation time ϵ is given by

$$A(q_n, q_{n+1}; \epsilon) = (2\pi\epsilon)^{-\frac{1}{2}}\ \ e^{-S_n^*}$$

- Ideal discretized action S^* is the sum of terms S_n^*

Ideal discretization (2)

- In general case, the ideal discretized action can be written as

$$S_n^* = \frac{\delta_n^2}{2\epsilon} + \epsilon W_n \,,$$

where W is the effective potential which contains $V(\bar{q}_n)$ and corrections

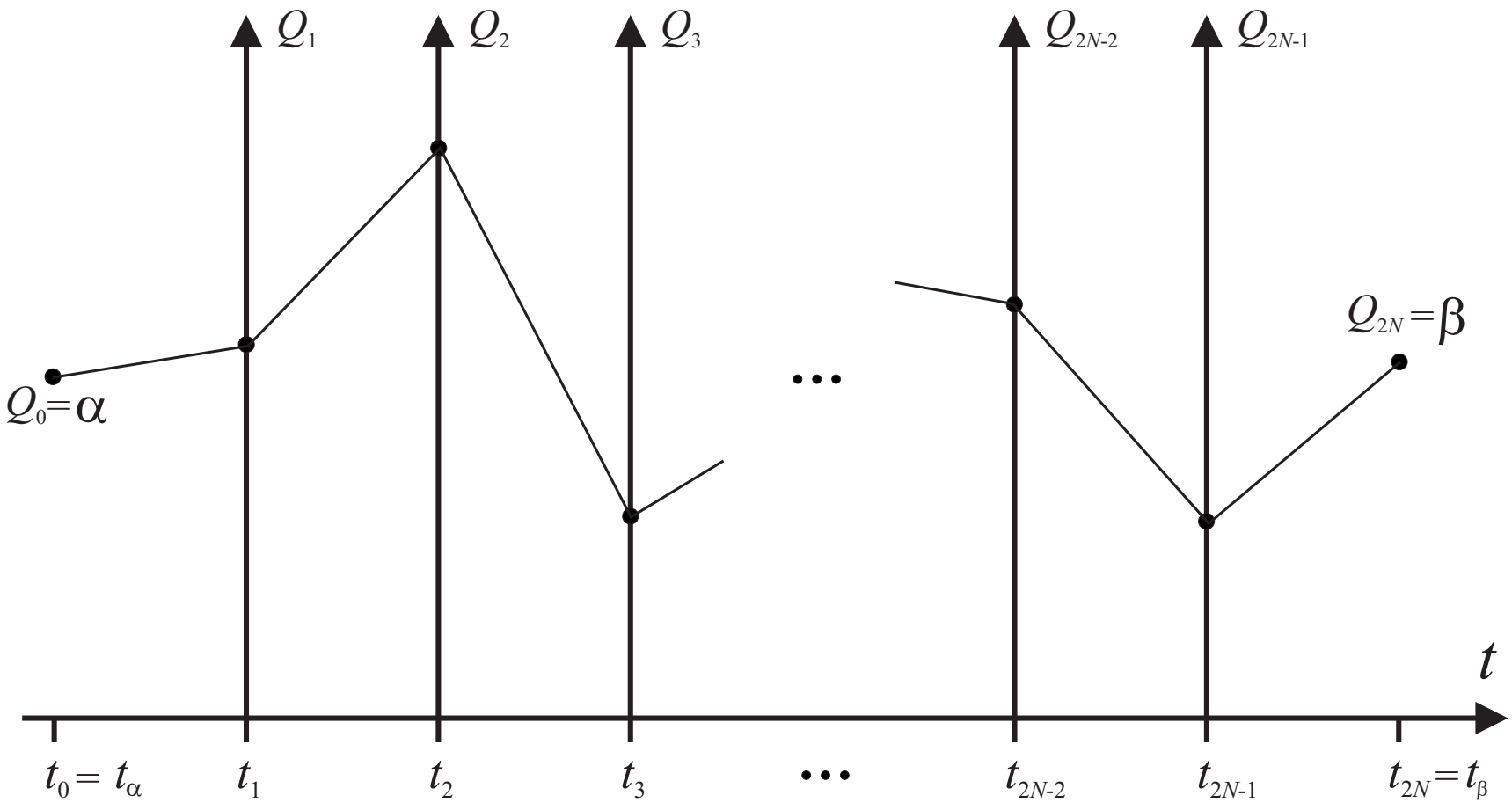
- From the definition of the ideal discretized action it follows

$$W_n = W(\delta_n, \bar{q}_n; \epsilon)$$

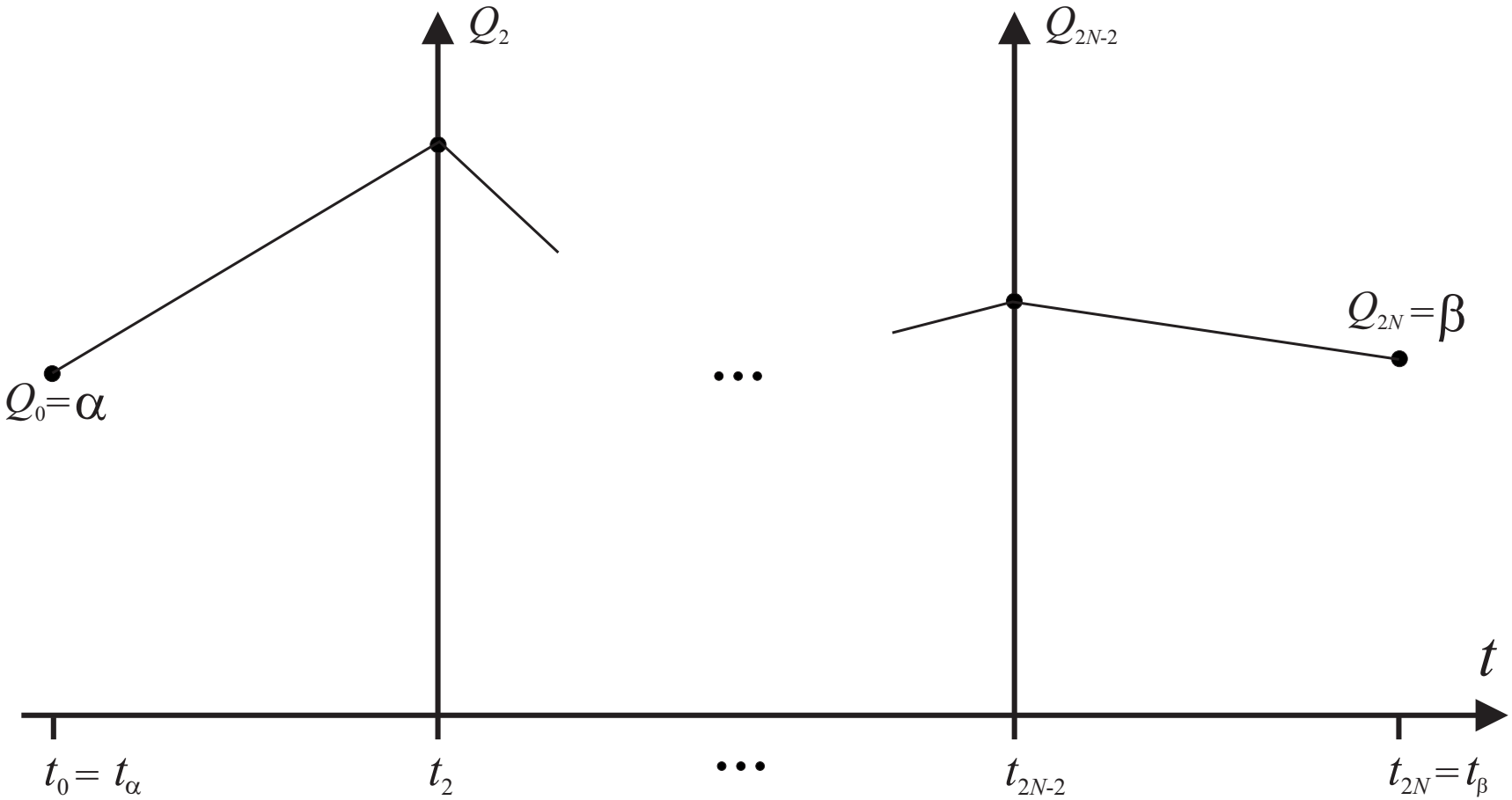
- From the reality of imaginary-time amplitudes, i.e. from the hermiticity of real-time amplitudes we obtain

$$W(\delta_n, \bar{q}_n; \epsilon) = W(-\delta_n, \bar{q}_n; \epsilon)$$

Relation between different discretizations (1)



Relation between different discretizations (2)



Relation between different discretizations (3)

- If we integrate out all odd-numbered coordinates, for a given discretized $2N$-action we get the effective N-action

$$e^{-\widetilde{S}_N} = \left(\frac{2}{\pi\epsilon_N}\right)^{\frac{N}{2}} \int dx_1 \cdots dx_N \; e^{-S_{2N}}$$

- However, if we use the ideal discretized action, then we get

$$e^{-S^*_N} = \left(\frac{2}{\pi\epsilon_N}\right)^{\frac{N}{2}} \int dx_1 \cdots dx_N \; e^{-S^*_{2N}}$$

Integral equation for the effective action

- From previous relation we obtain integral equation for the effective potential in the form

$$e^{-\epsilon_N W(\delta_n,\bar{q}_n;\epsilon_N)} = \left(\frac{2}{\pi\epsilon_N}\right)^{\frac{1}{2}} \int_{-\infty}^{+\infty} dy\, e^{-\frac{2}{\epsilon_N}y^2} \times G\left(\bar{q}_n + y; q_n, q_{n+1}, \frac{\epsilon_N}{2}\right),$$

where function G is defined as

$$-\frac{2}{\epsilon_N} \ln G(x; q_n, q_{n+1}, \epsilon_N) = W\left(q_{n+1} - x, \frac{q_{n+1}+x}{2}; \epsilon_N\right) + W\left(x - q_n, \frac{x+q_n}{2}; \epsilon_N\right)$$

Euler's summation formula (1)

- For ordinary integrals Euler's summation formula reads

$$I[f] = \int_0^T f(t)dt = \sum_{n=1}^{N} f(t_n)\epsilon_N - \frac{\epsilon_N}{2}\sum_{n=1}^{N} f'(t_n)\epsilon_N + \frac{\epsilon_N^2}{6}\sum_{n=1}^{N} f''(t_n)\epsilon_N + \dots$$

- $I[f]$ is now written as a series in time step ϵ_N,

$$I[f] = I_N[f^{(p)}] + O(\epsilon_N^p)\,,$$

where $f^{(p)}$ is the corresponding initial part of the ideal f^*

- Using W, we will derive Euler's summation formula for path integrals

Euler's summation formula (2)

- When we expand function G in a series in the first argument around $\bar{q}_n$, we get the following equation for W

$$W(\delta_n, \bar{q}_n; \epsilon_N) = -\frac{1}{\epsilon_N} \ln \left[\sum_{k=0}^{\infty} \frac{G^{(2k)}\left(\bar{q}_n; q_n, q_{n+1}, \frac{\epsilon_N}{2}\right)}{(2k)!!} \left(\frac{\epsilon_N}{4}\right)^k \right]$$

- Further application of asymptotic expansion makes use of the expansion of the ideal effective potential in a series

$$W(\delta_n, \bar{q}_n; \epsilon_N) = \sum_{k=0}^{\infty} \delta_n^{2k} \, g_k(\bar{q}_n; \epsilon_N)$$

- From the equation for W we get a system of differential equations for functions g_k

Euler's summation formula (3)

- If we expand functions g_k into series in the time step ϵ

$$g_k(\bar{q}_n;\epsilon_N) = \sum_{m=0}^{p-k-1} \epsilon_N^m \, g_{km}(\bar{q}_n) \qquad (k = 0, \ldots, p-1)$$

  we obtain a system of equations that is easily decoupled and can be solved in functions g_k
- Note that in the above expression the sum is limited according to the consistency condition which follows from the diffusion relation $\delta^2 \propto \epsilon$
- Boundary condition for the above system is $g_{00} = V$, obtained from limits $\delta_n^2 \to 0$ and $\epsilon_N \to 0$, in which W reduces to

$$W(0, \bar{q}_n; 0) = V(\bar{q}_n)$$

Euler's summation formula (4)

- To level $p = 3$ we get

$$g_0(\bar{q}_n;\epsilon_N) = V(\bar{q}_n) + \epsilon_N \frac{V''(\bar{q}_n)}{12} + \epsilon_N^2 \left[-\frac{V'(\bar{q}_n)^2}{24} + \frac{V^{(4)}(\bar{q}_n)}{240} \right]$$

$$g_1(\bar{q}_n;\epsilon_N) = \frac{V''(\bar{q}_n)}{24} + \epsilon_N \frac{V^{(4)}(\bar{q}_n)}{480}$$

$$g_2(\bar{q}_n;\epsilon_N) = \frac{V^{(4)}(\bar{q}_n)}{1920}$$

- Ideal effective action on the convergence level p is given as

$$S_N^{(p)} = \sum_{n=0}^{N-1} \left[\frac{\delta_n^2}{2\epsilon_N} + \epsilon_N \sum_{k=0}^{p-1} \delta_n^{2k}\, g_k(\bar{q}_n;\epsilon_N) \right]$$

- This ensures the improved convergence
$A_N^{(p)}(\alpha,\beta;T) = A(\alpha,\beta;T) + O(\epsilon_N^p)$

Recursive approach

- Gaussian halving is developed and applicable for one-particle one-dimensional systems only
- For many-body systems in arbitrary dimensions we have developed two equivalent approaches
- First is based on direct calculation of ϵ-expansion of short-time amplitudes, expressed as expectation values of the corresponding free theory
  - following the original idea from the book by H. Kleinert
- Here we present second approach, based on solving recursive relations for the discretized action, derived from Schrödinger's equation for amplitudes.
- This approach is by far the most efficient, both for many-body and one-body systems.

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 $x = \delta/2$, $\bar{x} = (q + q')/2$, $V_\pm = V(\bar{x} \pm x)$

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

Recursive relations (1)

- 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

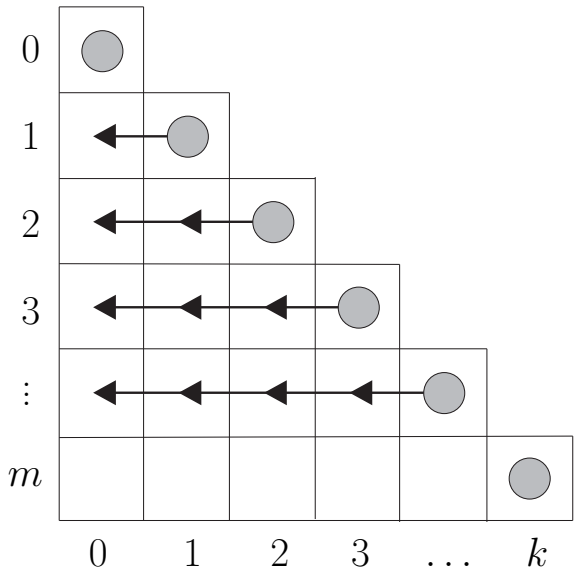
$$\begin{aligned}8\,(m+k+1)\,W_{m,k} = {}& \bar{\partial}^2 W_{m-1,k} + \partial^2 W_{m,k+1} - \\ & - \sum_{l=0}^{m-2}\sum_{r}(\bar{\partial}W_{l,r})\cdot(\bar{\partial}W_{m-l-2,k-r}) - \\ & - \sum_{l=1}^{m-2}\sum_{r}(\partial W_{l,r})\cdot(\partial W_{m-l-1,k-r+1})\end{aligned}$$

Recursive relations (2)

- Diagonal coefficients are easily obtained from recursive relations

$$W_{m,m} = \frac{1}{(2m+1)!}(x \cdot \bar{\partial})^{2m} V$$

- Off-diagonal coefficients are obtained by applying recursive relations in the following order



Effective actions for many-body systems

- To level $p = 3$, effective action is given by

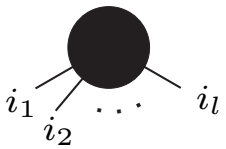
$$
\begin{aligned}
W_{0,0} &= V \\
W_{1,1} &= \frac{1}{6}\,(x\cdot\bar{\partial})^2 V \\
W_{1,0} &= \frac{1}{12}\bar{\partial}^2 V \\
W_{2,2} &= \frac{1}{120}\,(x\cdot\bar{\partial})^4 V \\
W_{2,1} &= \frac{1}{120}(x\cdot\bar{\partial})^2\,\bar{\partial}^2 V \\
W_{2,0} &= \frac{1}{240}\,\bar{\partial}^4 V - \frac{1}{24}\,(\bar{\partial}V)\cdot(\bar{\partial}V)
\end{aligned}
$$

Diagrammatic form of effective actions (1)

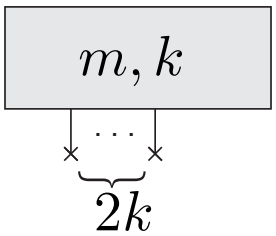
- Derived recursive relations can be represented in a diagrammatic form if we introduce

$$\delta_{ij} = \quad i \text{ ——— } j \ , \qquad x_i = \quad \times\!\!\longleftarrow \ i$$

$$\bar{\partial}_{i_1}\bar{\partial}_{i_2}\cdots\bar{\partial}_{i_l}V =$$



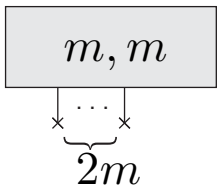
$$, \qquad W_{m,k} =$$



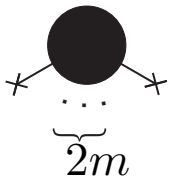
$$.$$

- Diagrammatic form of diagonal coefficients

$$W_{m,m} =$$



$$= \frac{1}{(2m+1)!}$$



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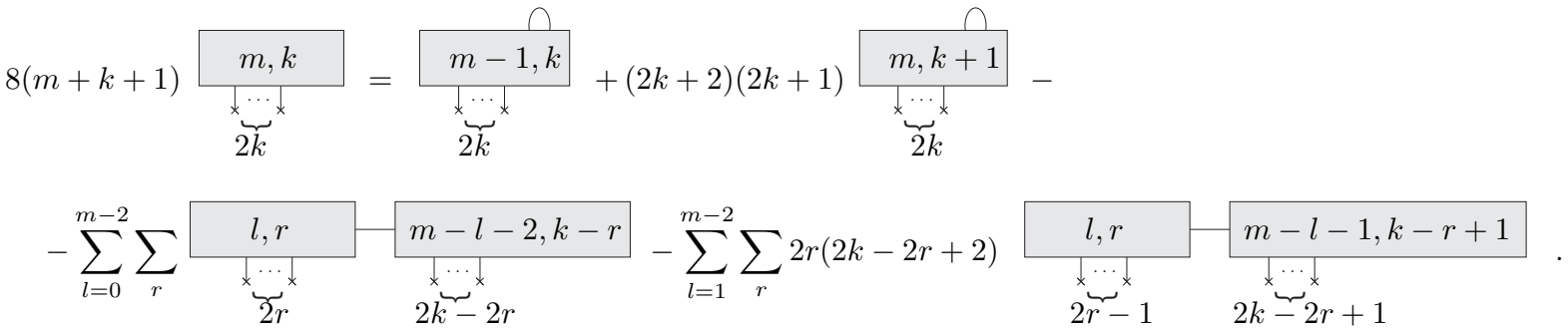
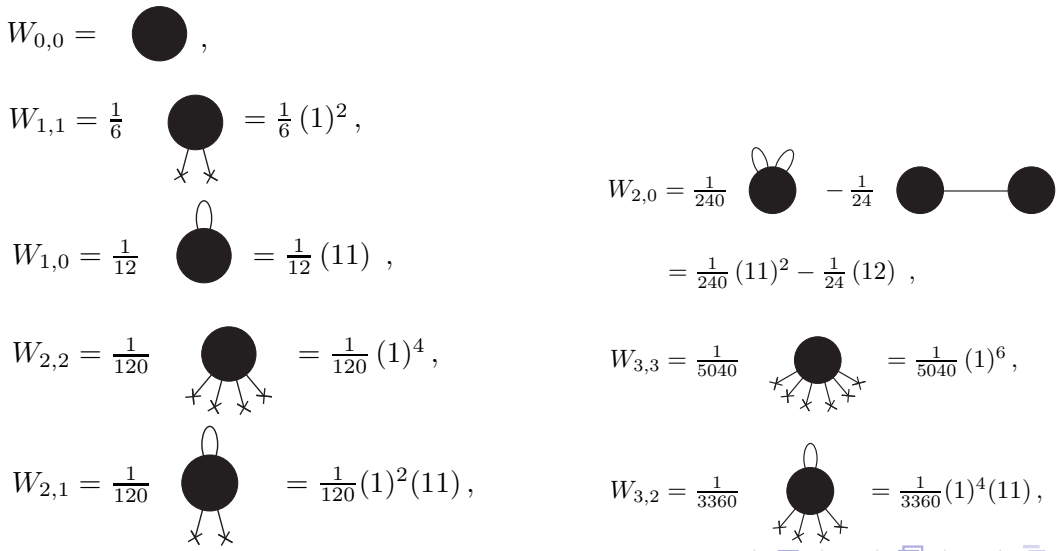
Diagrammatic form of effective actions (2)

- Diagrammatic form of recursive relations



- Solutions to level $p = 3$



Ideal Bose gases (1)

- Good approximation for weakly-interacting dilute gases
- Bose-Einstein condensates usually realized in harmonic magneto-optical traps
- Fast-rotating Bose-Einstein condensates extensively studied - 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)]

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 profile 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}

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

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

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

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

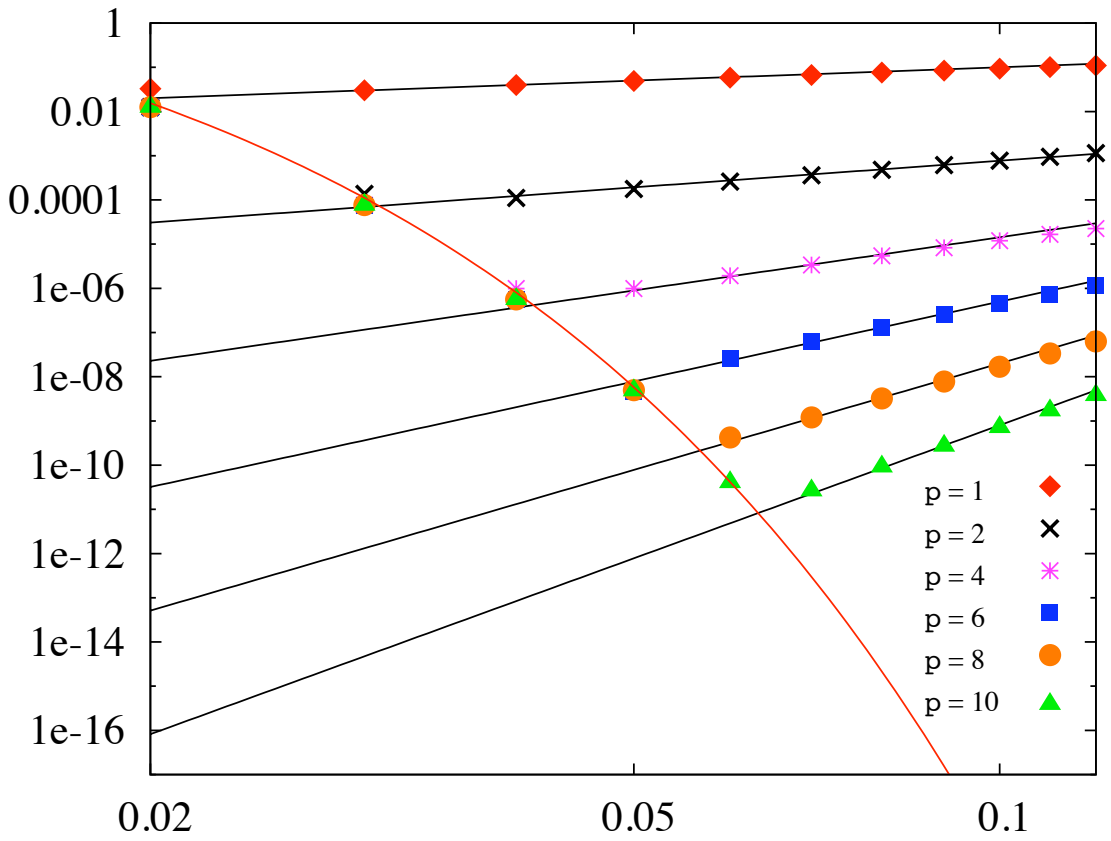
- The condensation temperature T_c is thus defined by the condition:

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

Energy eigenvalues and eigenstates (1)

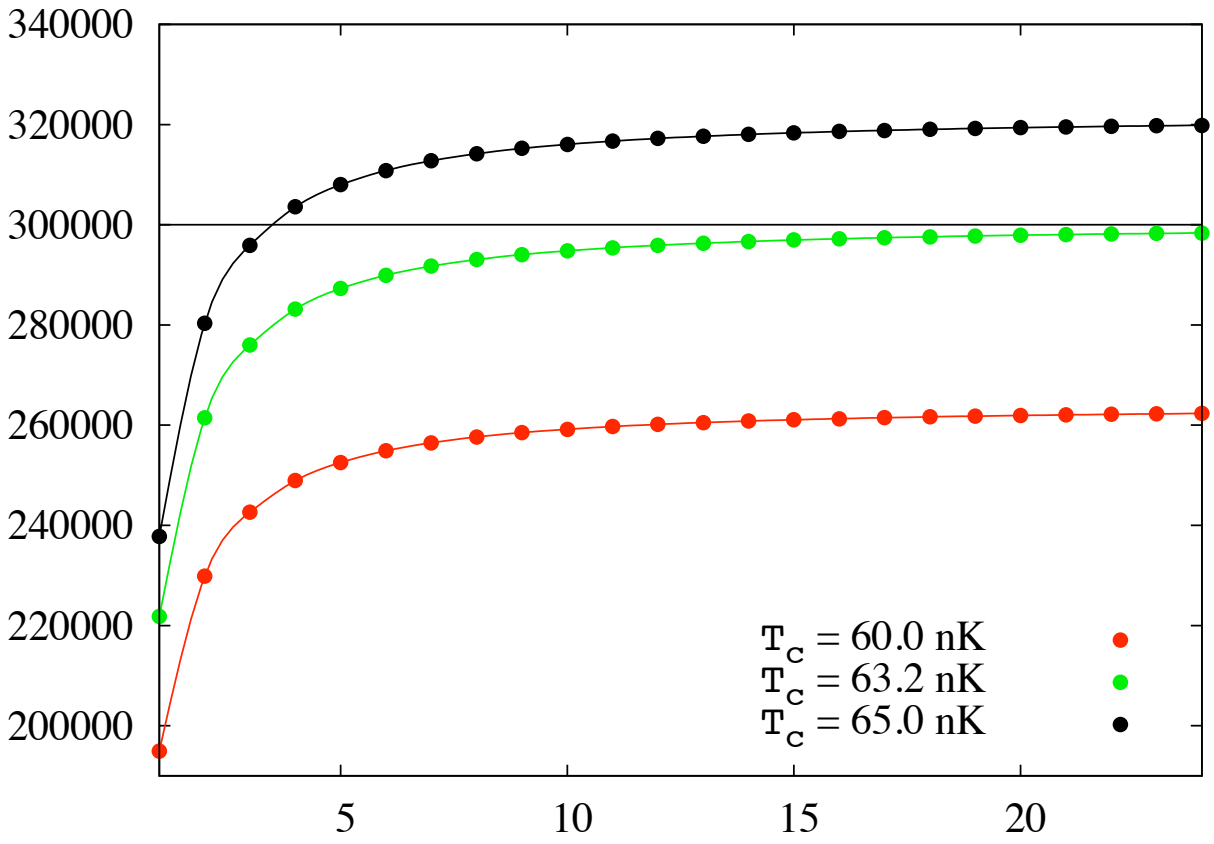
- Single-particle eigenvalues and eigenstates are sufficient for the calculation of BEC condensation temperature
- The most efficient approach for low-dimensional systems is direct diagonalization of space-discretized propagator $e^{-\epsilon \hat{H}}$, where ϵ is appropriately chosen artificial short-time of propagation ($N = 1$ 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

Energy eigenvalues and eigenstates (2)



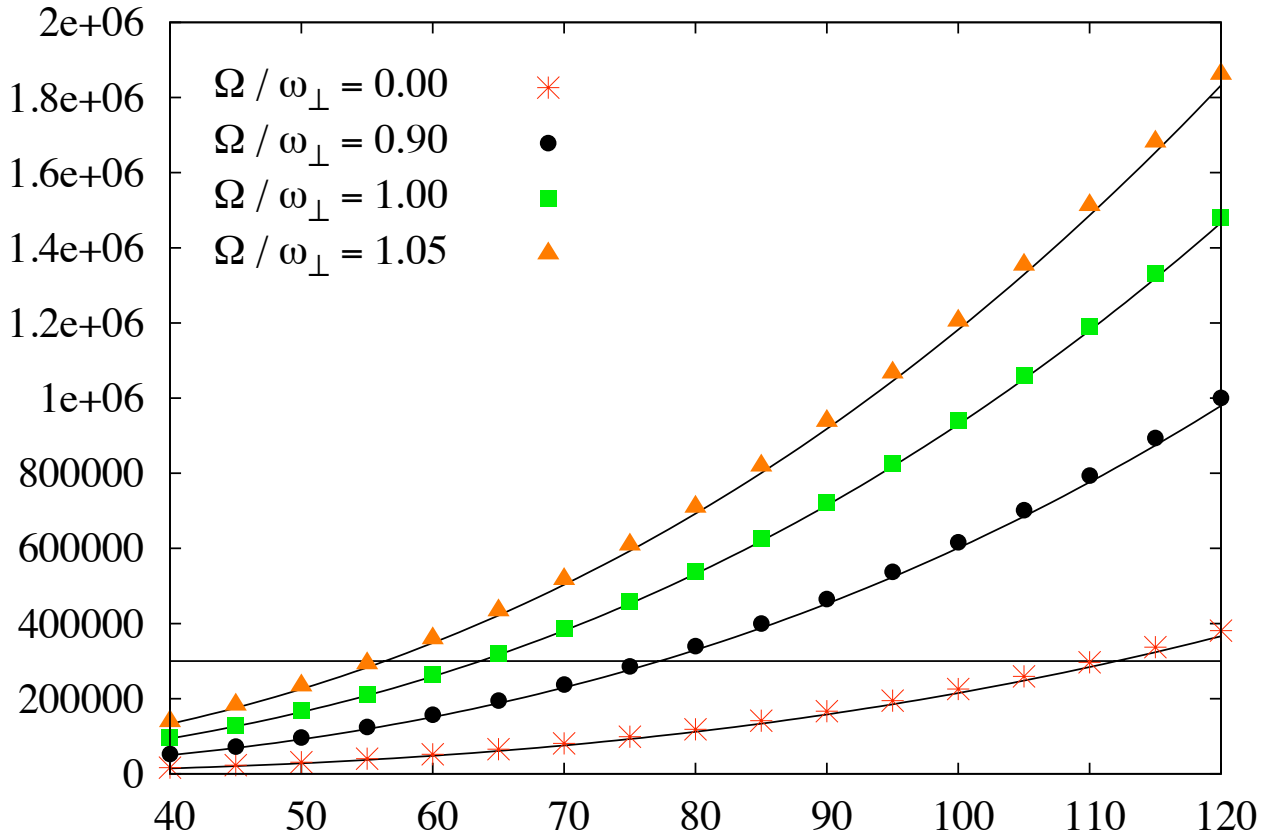
Deviations from the exact ground-state energy vs. ϵ for V_{BEC} (critical rotation). The error is proportional to ϵ^p. The red curve is the discretization error (analytically known).

Calculation of the condensation temperature (1)



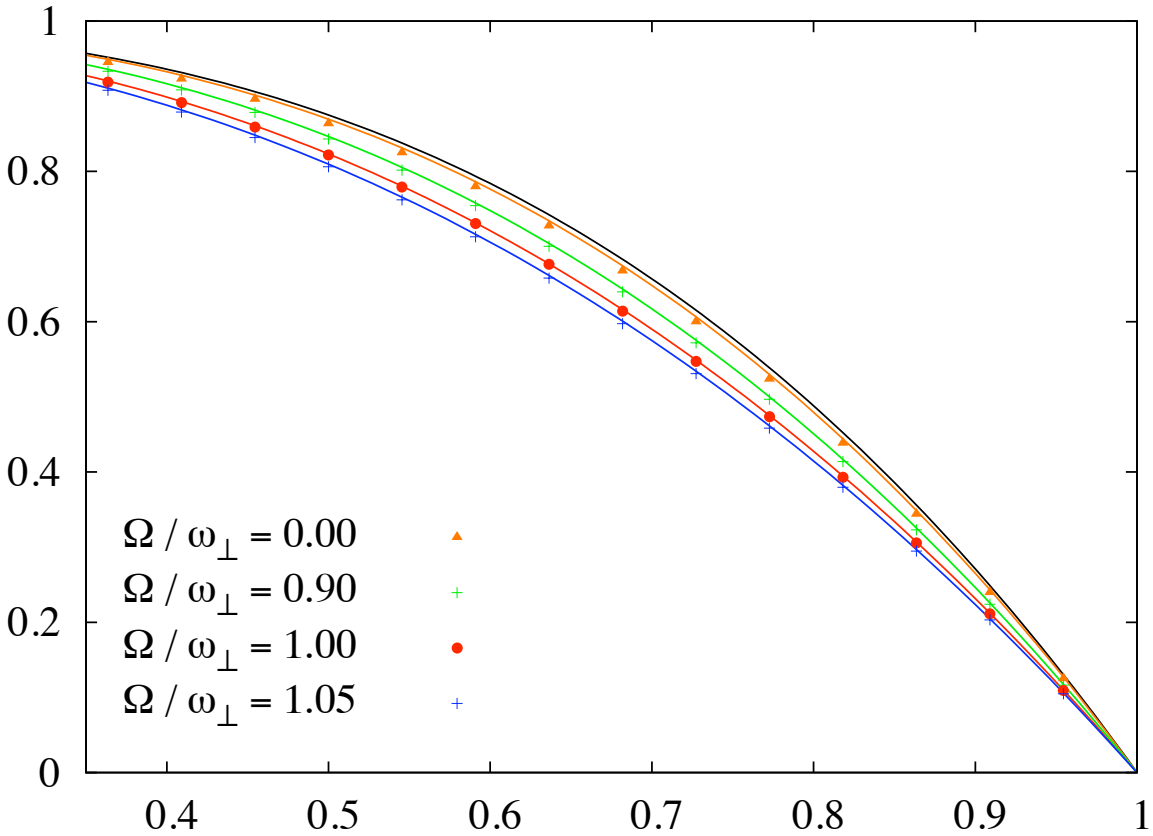
Partial sums $\sum_{m=1}^{M}(e^{m\beta E_0}\mathcal{Z}_1(m\beta)-1)$ as a function of M for critical rotation, obtained with $p=18$ effective action.

Calculation of the condensation temperature (2)



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).

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 $n \geq 1$,

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

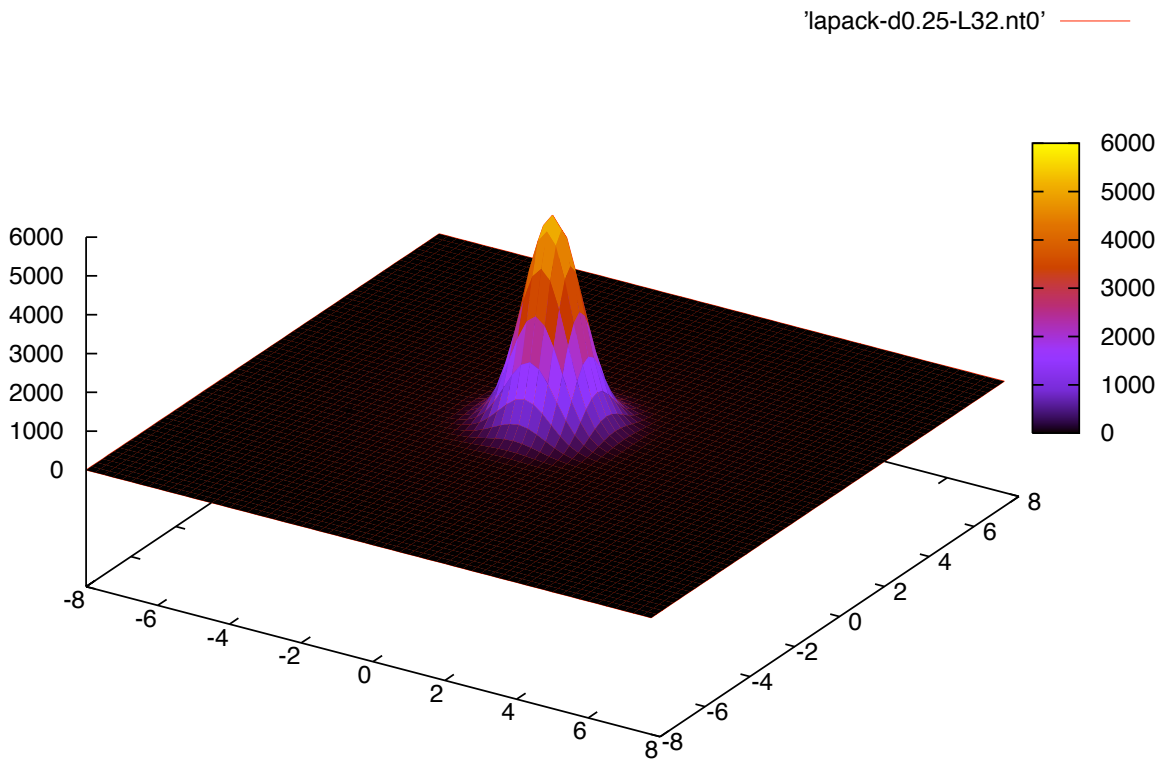
Density profiles of Bose-Einstein condensates (2)

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

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

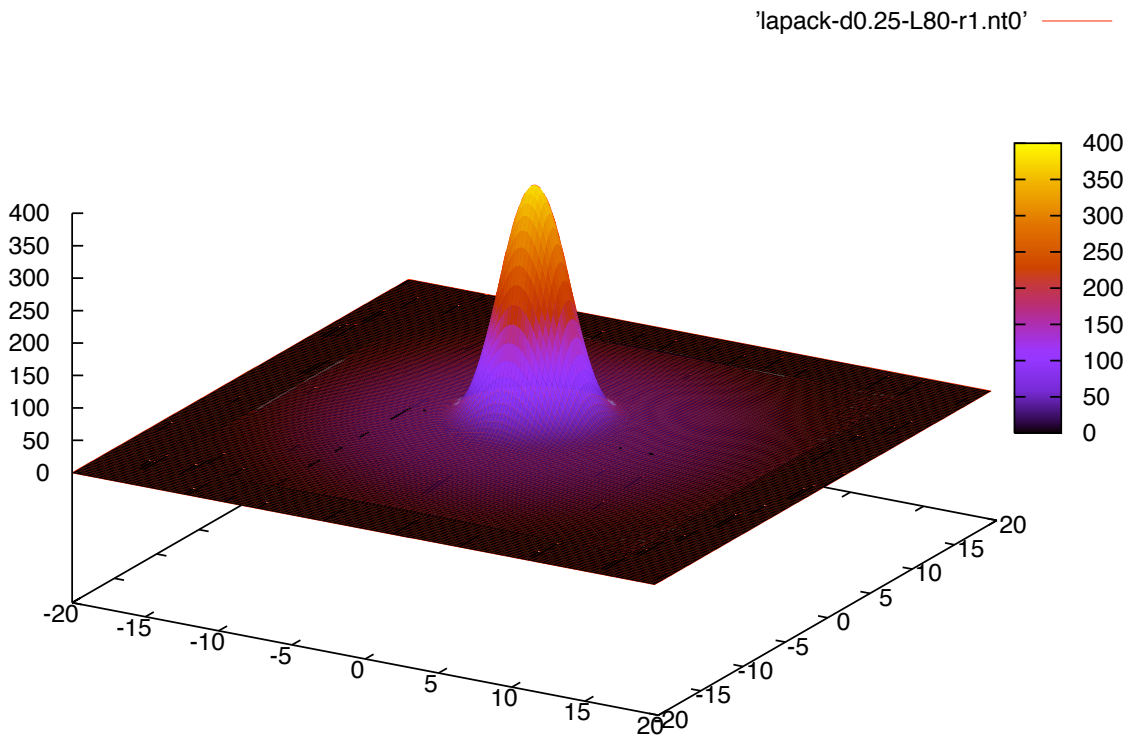
  where $A(\vec{r},0;\vec{r},m\beta\hbar)$ represents the (imaginary-time) amplitude for one-particle transition from the position $\vec{r}$ in $t=0$ to the position $\vec{r}$ in $t=m\beta\hbar$
- Both definitions are mathematically equivalent
- The first one is more suitable for low temperatures, while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

Density profiles of Bose-Einstein condensates (3)



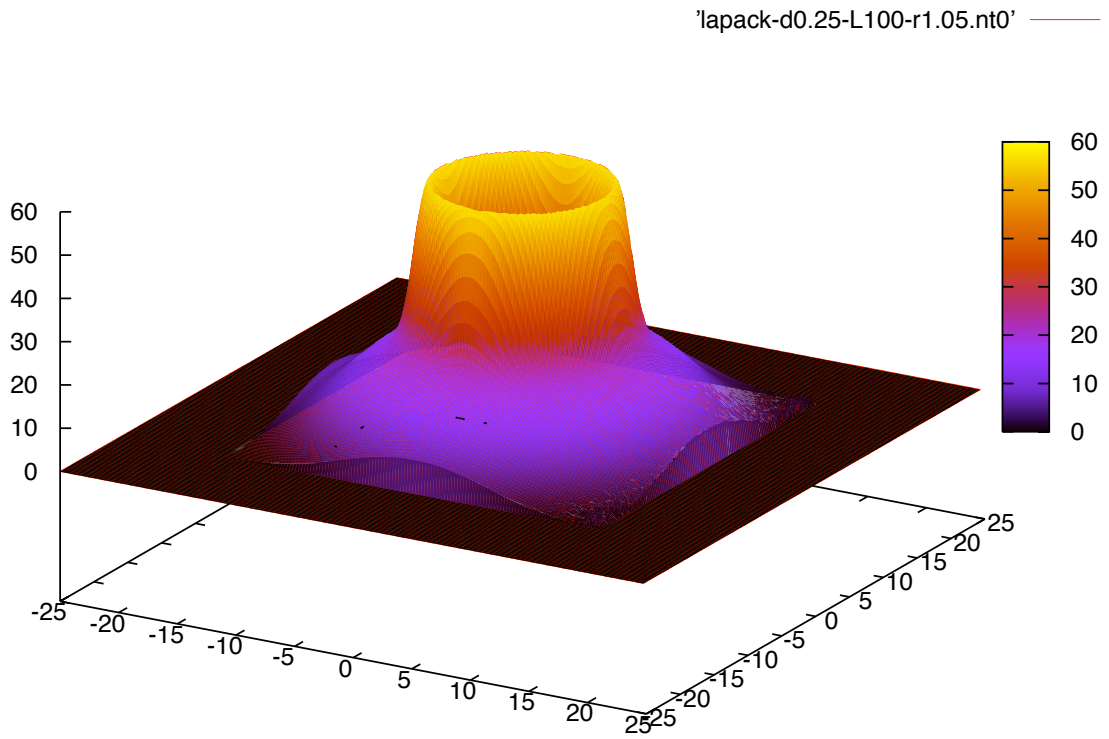
Density profile in $x-y$ plane for the condensate without rotation. $T = 50$ nK $< T_c = 110.4$ nK ($\beta = 6.2 \times 10^{-2}$). The linear size of the profile is 20 μm.

Density profiles of Bose-Einstein condensates (4)



Density profile in $x-y$ plane for the condensate at critical rotation. $T = 50$ nK $< T_c = 63.1$ nK ($\beta = 6.2 \times 10^{-2}$). The linear size of the profile is 54 μm.

Density profiles of Bose-Einstein condensates (5)



Density profile in $x-y$ plane for the condensate at overcritical rotation ($\Omega/\omega_\perp = 1.05$). $T = 50$ nK $< T_c = 55.5$ nK ($\beta = 6.2 \times 10^{-2}$). The linear size of the profile is 67 μm.

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 10 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

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

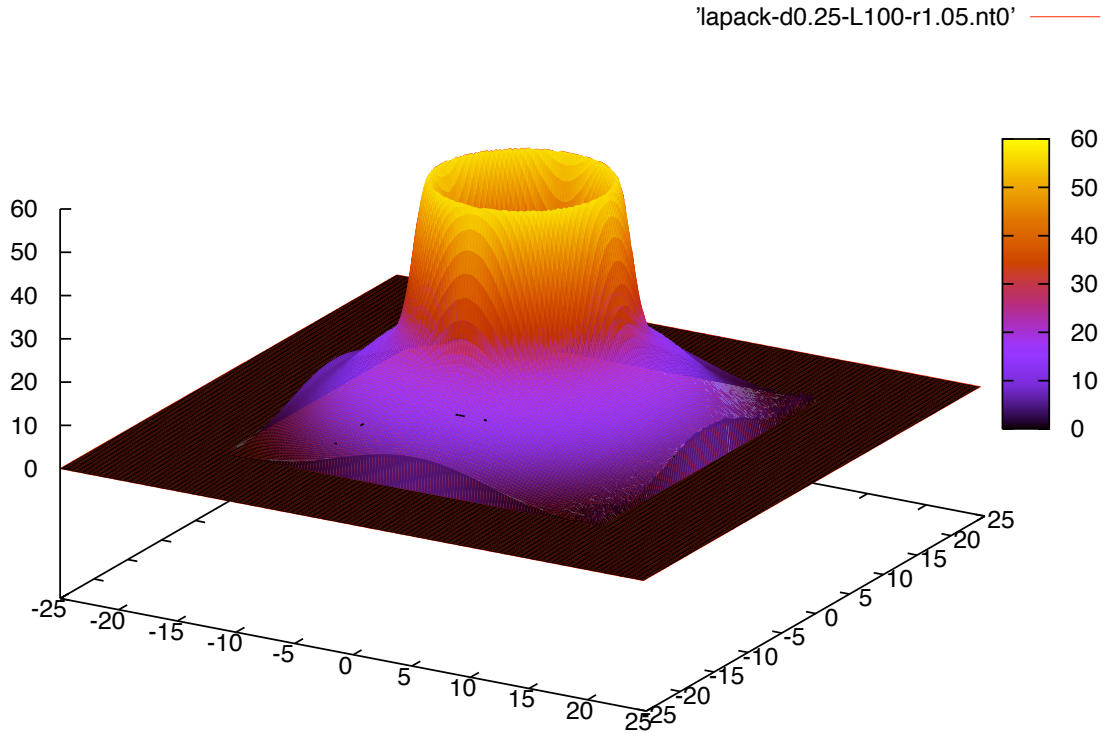
Time-of-flight graphs for BECs (2)

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

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

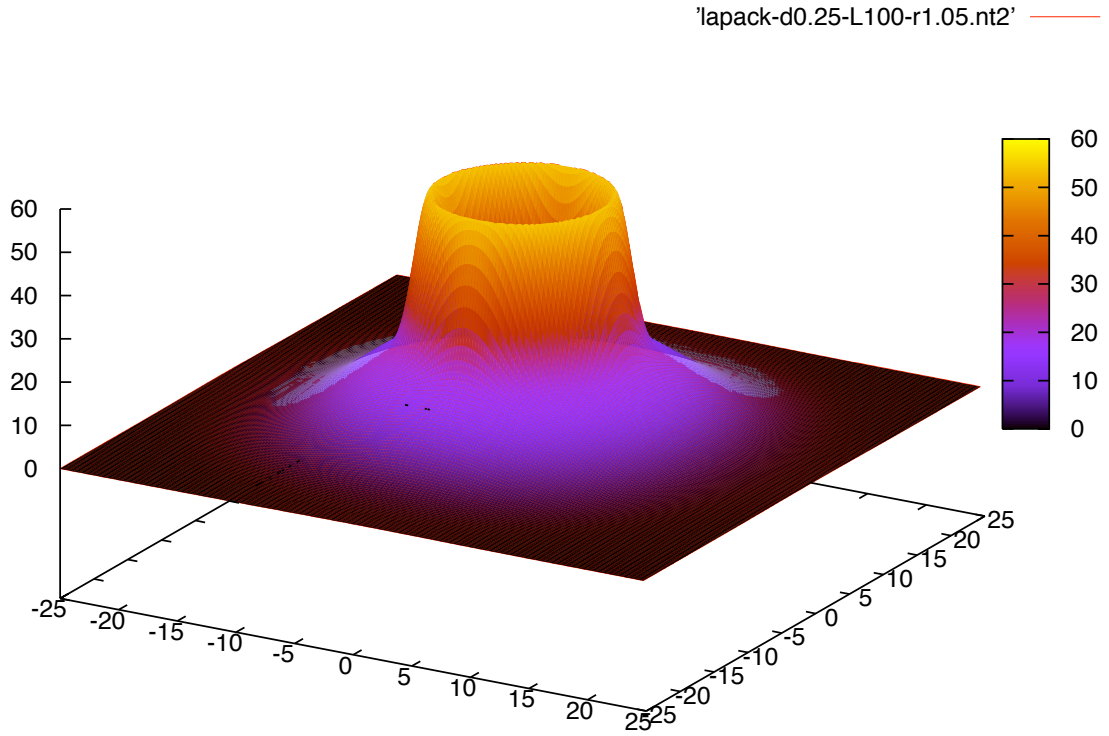
- In both approaches it is first necessary to calculate E_0 and $\psi_0(\vec{r})$ using direct diagonalization or some other method
- FFT is ideally suitable for numerical calculations of time-of-flight graphs

Time-of-flight graphs for BECs (3)



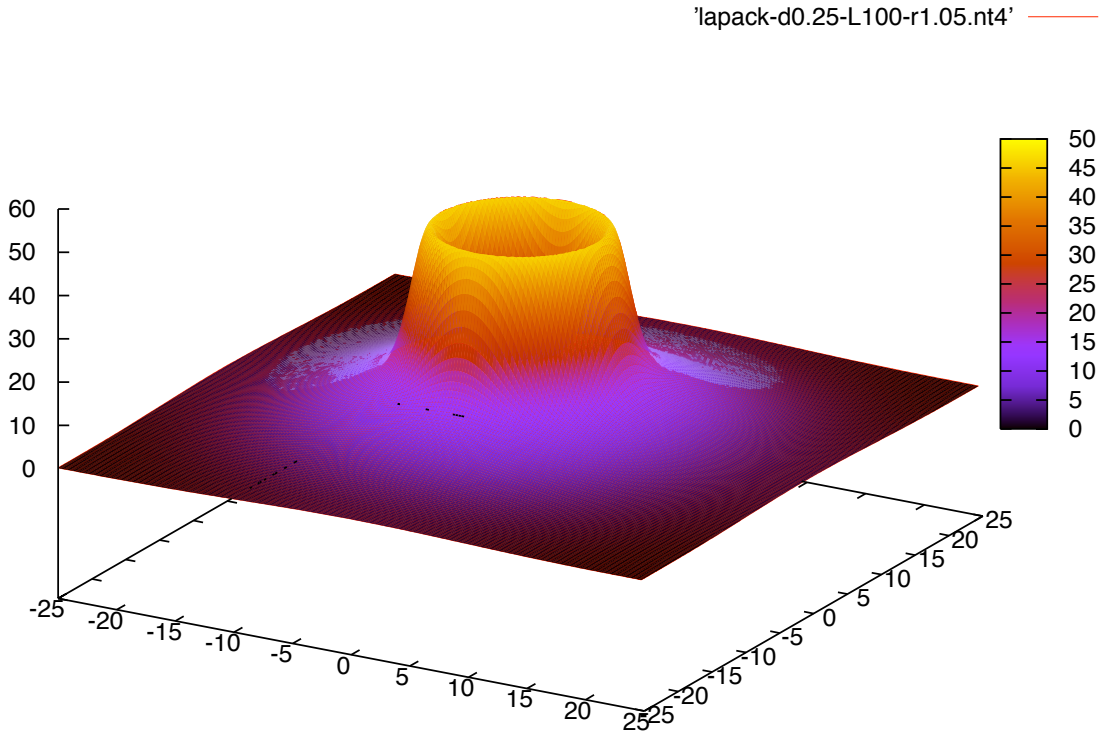
Time-of-flight graph at $t = 0$ ms in $x - y$ plane for the condensate at overcritical rotation ($\Omega/\omega_\perp = 1.05$). $T = 50$ nK $< T_c = 55.5$ nK ($\beta = 6.2 \times 10^{-2}$). The linear size of the profile is 67 μm.

Time-of-flight graphs for BECs (4)



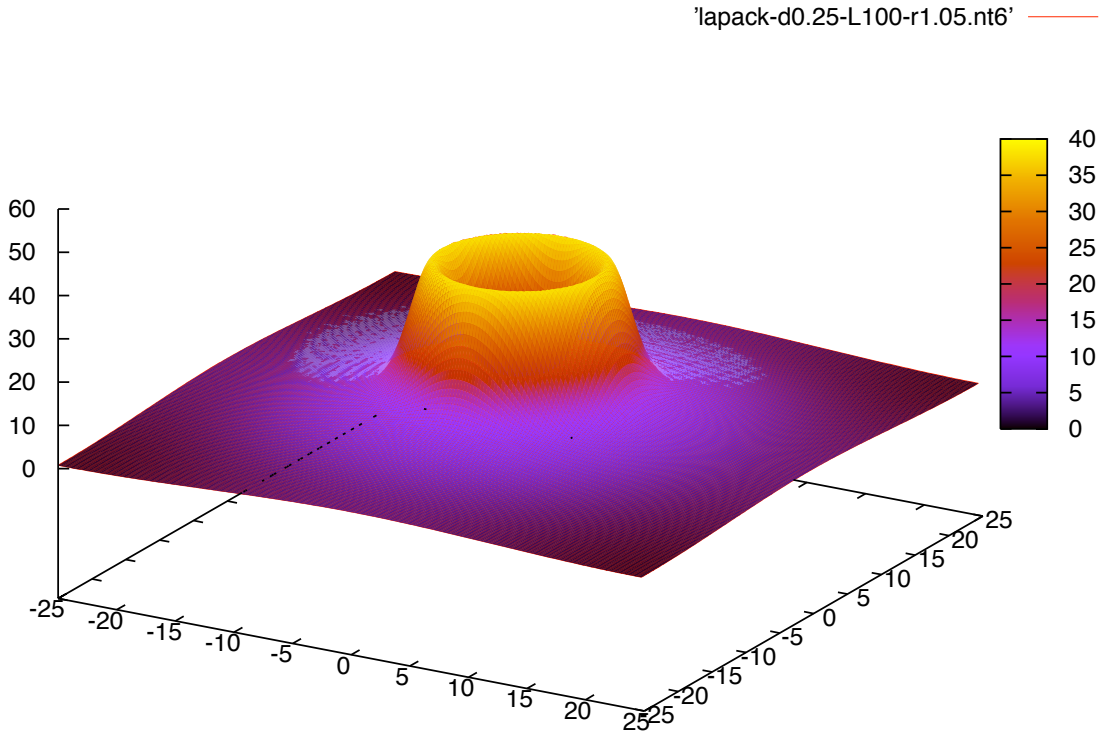
Time-of-flight graph at $t = 2$ ms in $x - y$ plane for the condensate at overcritical rotation ($\Omega/\omega_\perp = 1.05$). $T = 50$ nK $< T_c = 55.5$ nK ($\beta = 6.2 \times 10^{-2}$). The linear size of the profile is 67 μm.

Time-of-flight graphs for BECs (5)



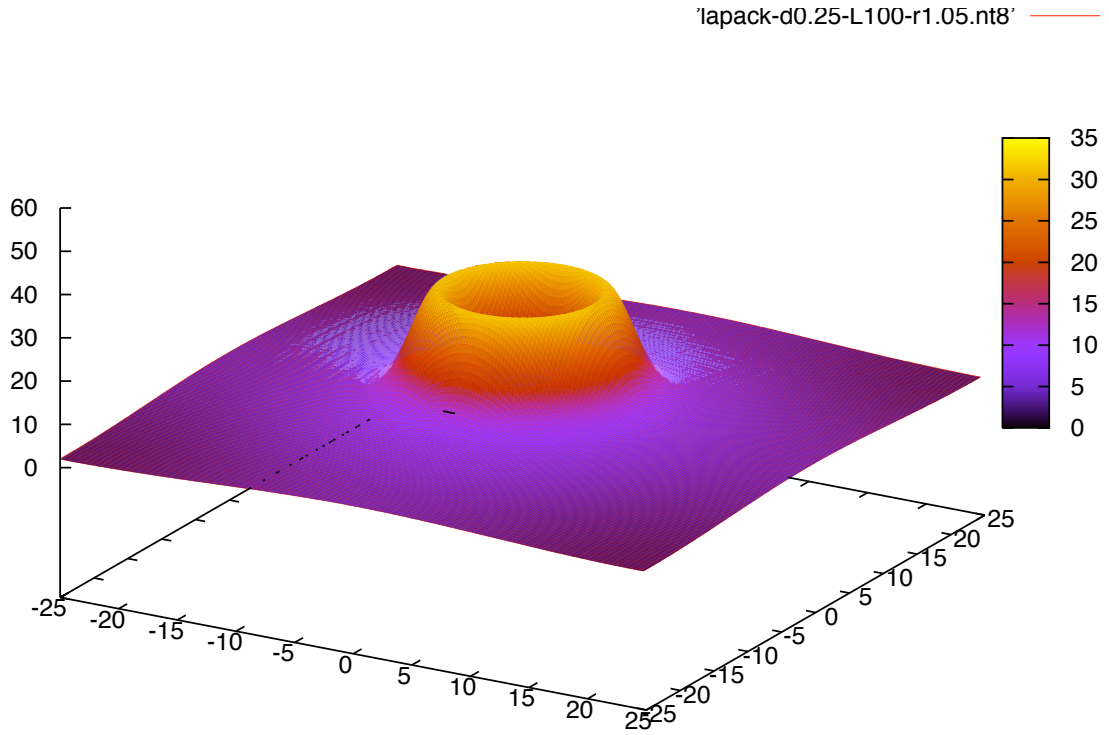
Time-of-flight graph at $t = 4$ ms in $x - y$ plane for the condensate at overcritical rotation ($\Omega/\omega_\perp = 1.05$). $T = 50$ nK $< T_c = 55.5$ nK ($\beta = 6.2 \times 10^{-2}$). The linear size of the profile is 67 μm.

Time-of-flight graphs for BECs (6)



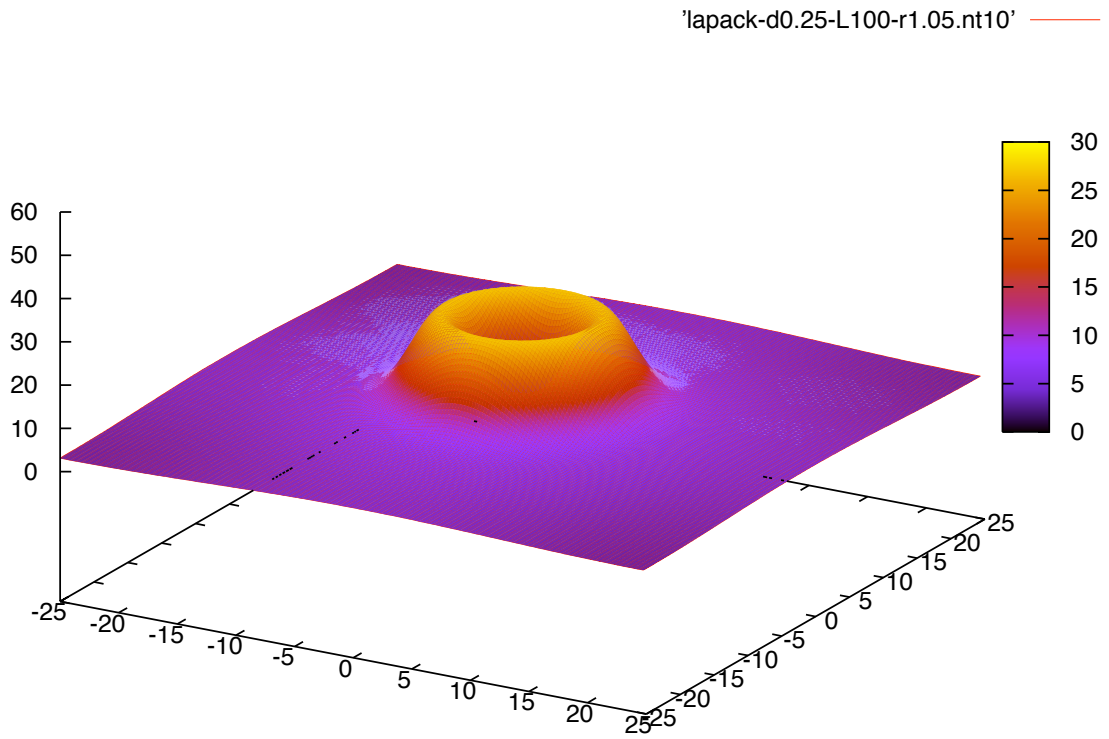
Time-of-flight graph at $t = 6$ ms in $x - y$ plane for the condensate at overcritical rotation ($\Omega/\omega_\perp = 1.05$). $T = 50$ nK $< T_c = 55.5$ nK ($\beta = 6.2 \times 10^{-2}$). The linear size of the profile is 67 μm.

Time-of-flight graphs for BECs (7)



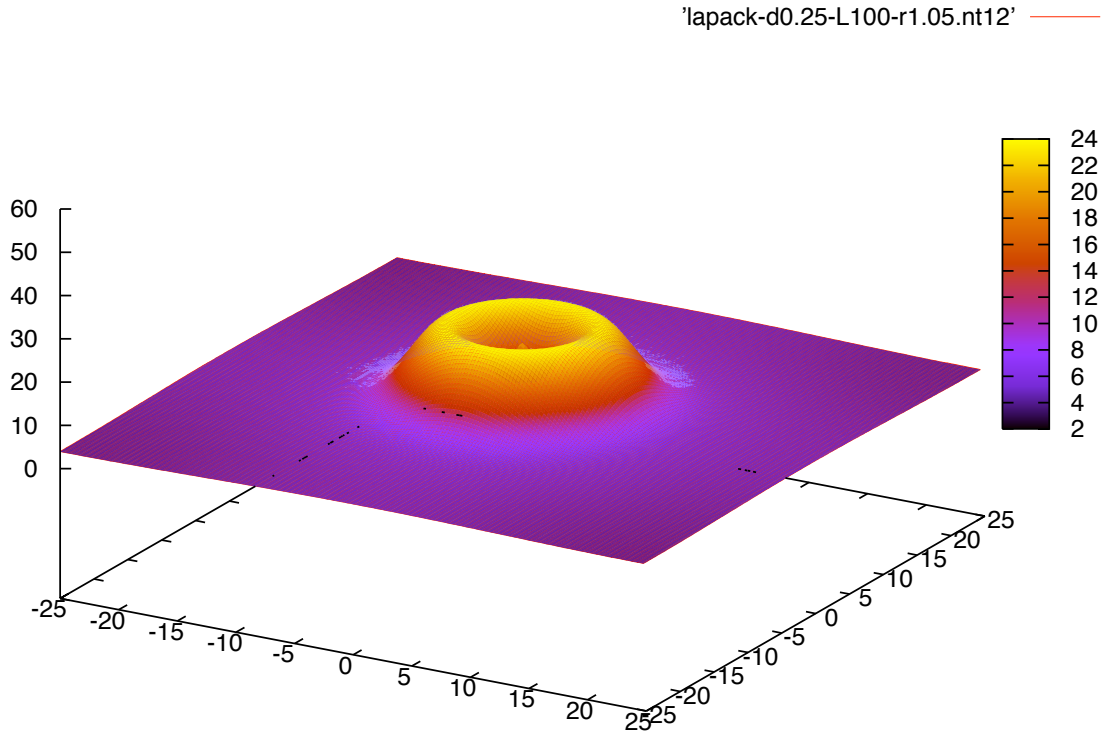
Time-of-flight graph at $t = 8$ ms in $x - y$ plane for the condensate at overcritical rotation ($\Omega/\omega_\perp = 1.05$). $T = 50$ nK $< T_c = 55.5$ nK ($\beta = 6.2 \times 10^{-2}$). The linear size of the profile is 67 μm.

Time-of-flight graphs for BECs (8)



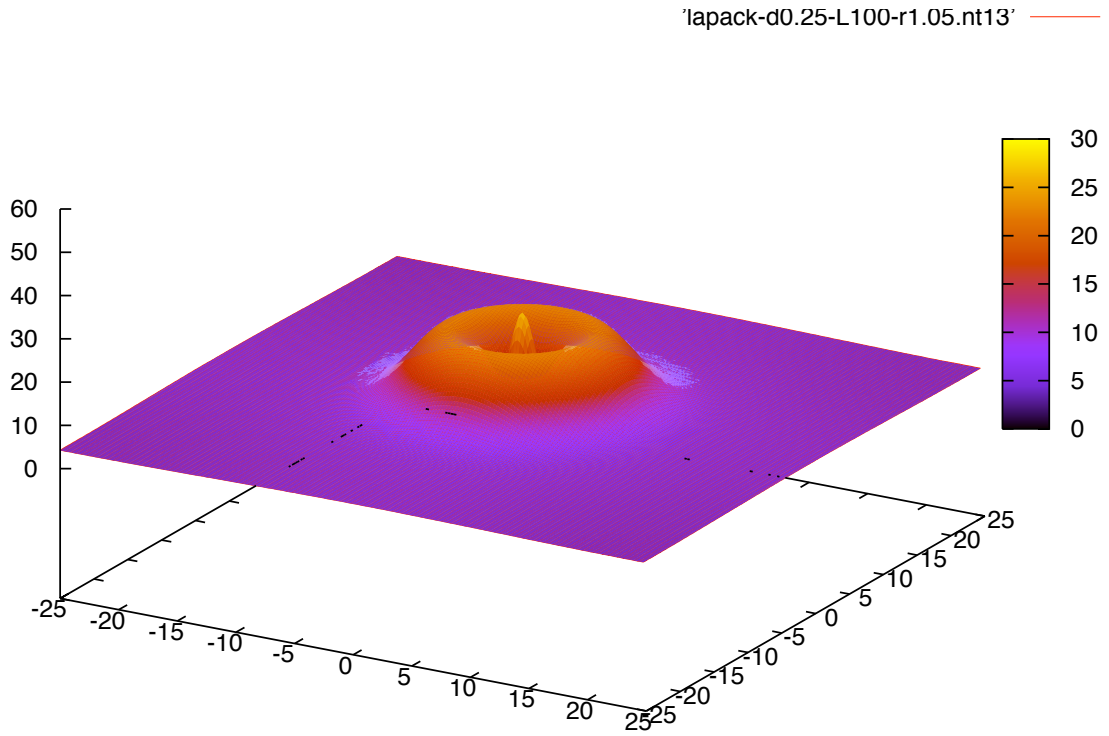
Time-of-flight graph at $t = 10$ ms in $x - y$ plane for the condensate at overcritical rotation ($\Omega/\omega_\perp = 1.05$). $T = 50$ nK $< T_c = 55.5$ nK ($\beta = 6.2 \times 10^{-2}$). The linear size of the profile is 67 μm.

Time-of-flight graphs for BECs (9)



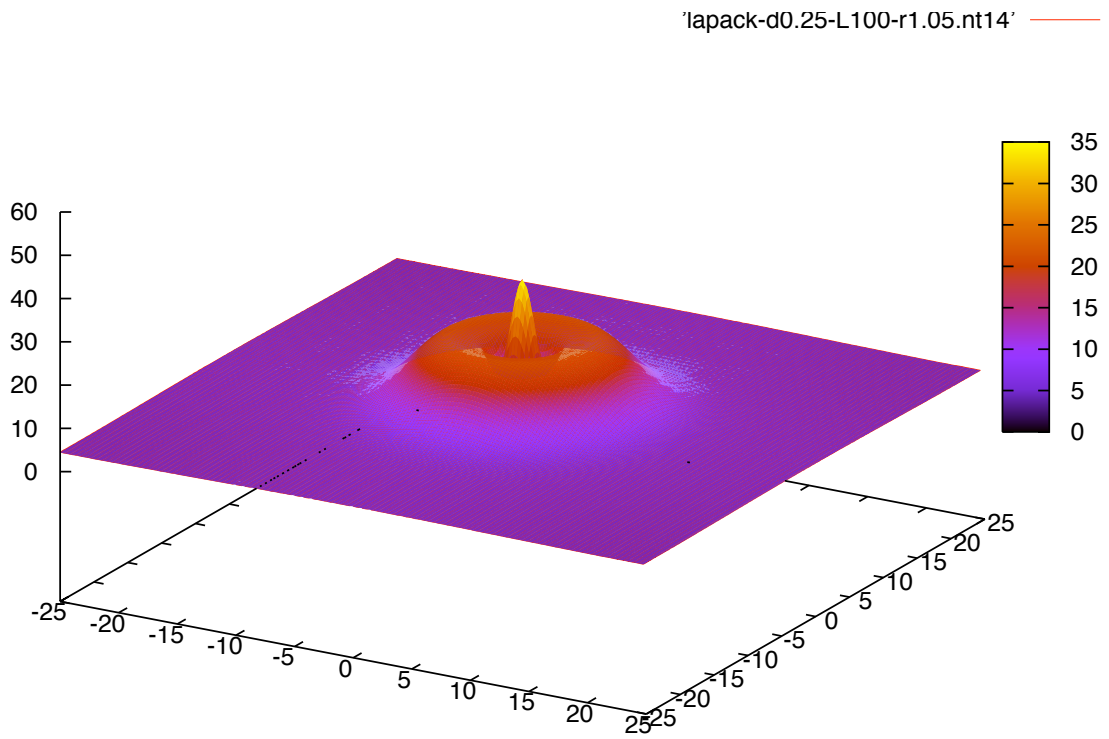
Time-of-flight graph at $t = 12$ ms in $x - y$ plane for the condensate at overcritical rotation ($\Omega/\omega_\perp = 1.05$). $T = 50$ nK $< T_c = 55.5$ nK ($\beta = 6.2 \times 10^{-2}$). The linear size of the profile is 67 μm.

Time-of-flight graphs for BECs (10)



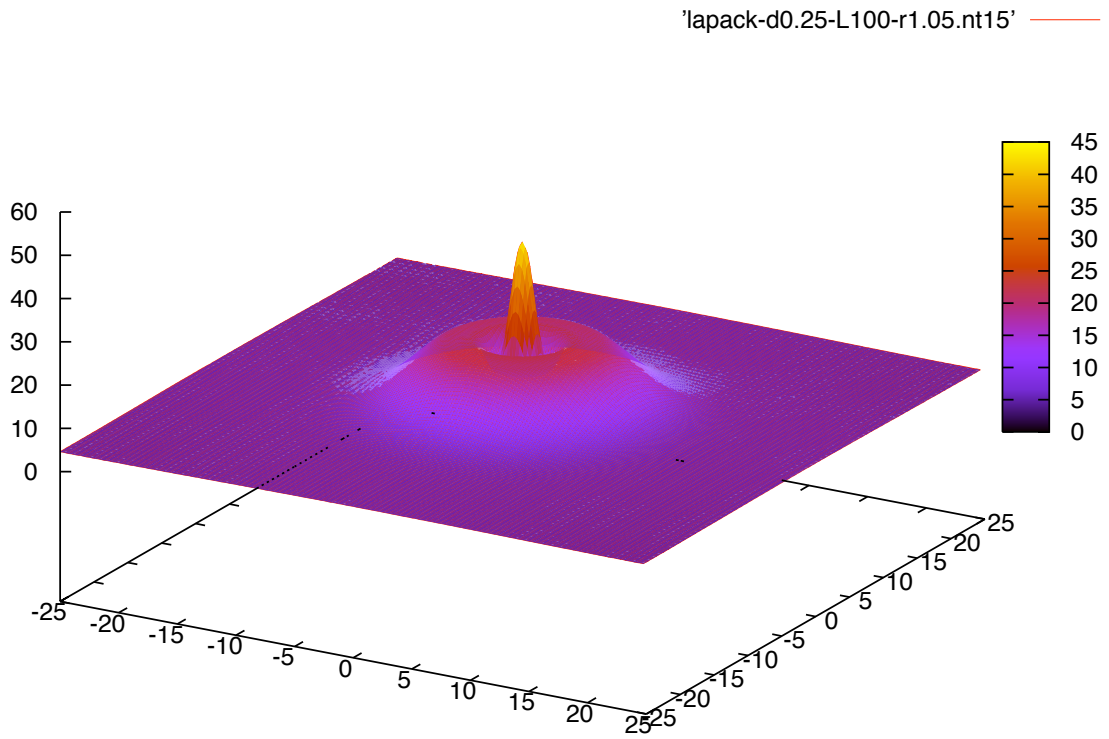
Time-of-flight graph at $t = 13$ ms in $x - y$ plane for the condensate at overcritical rotation ($\Omega/\omega_\perp = 1.05$). $T = 50$ nK $< T_c = 55.5$ nK ($\beta = 6.2 \times 10^{-2}$). The linear size of the profile is 67 μm.

Time-of-flight graphs for BECs (11)



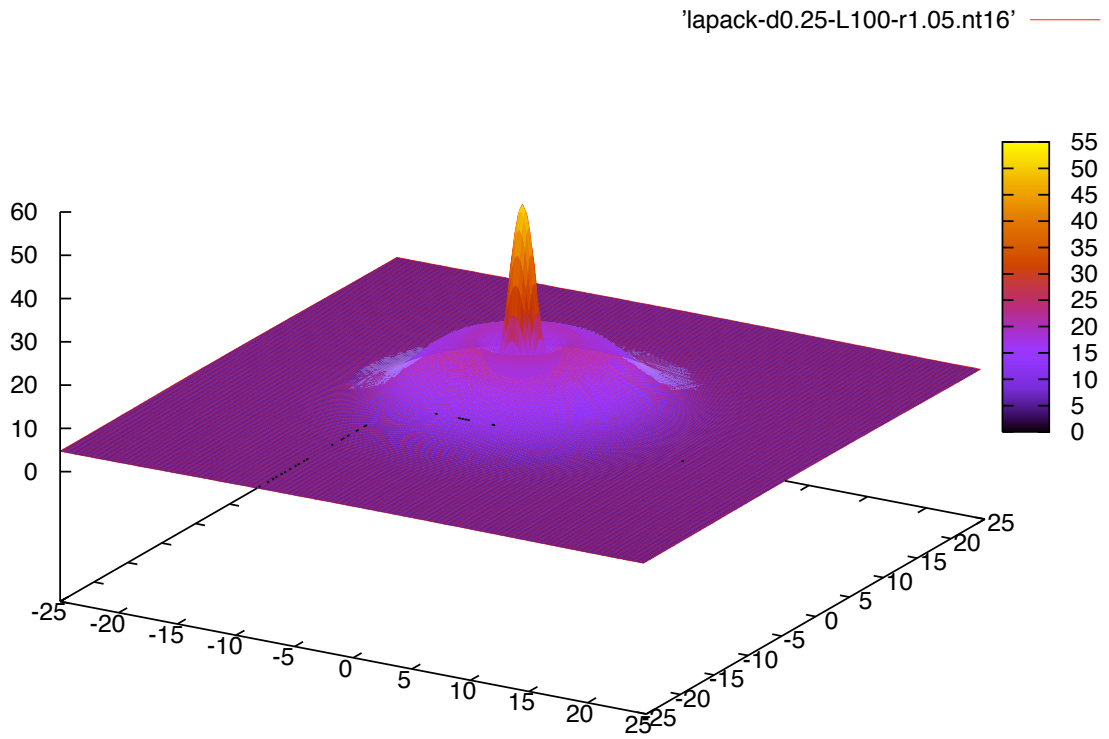
Time-of-flight graph at $t = 14$ ms in $x - y$ plane for the condensate at overcritical rotation ($\Omega/\omega_\perp = 1.05$). $T = 50$ nK $< T_c = 55.5$ nK ($\beta = 6.2 \times 10^{-2}$). The linear size of the profile is 67 μm.

Time-of-flight graphs for BECs (12)



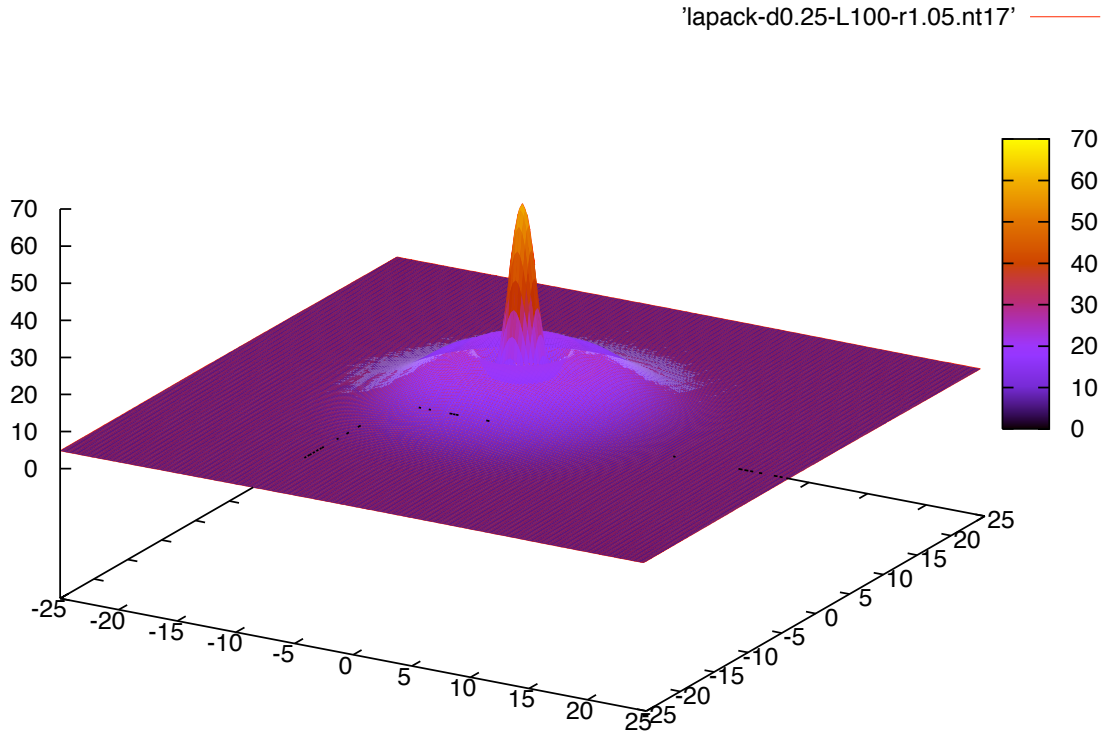
Time-of-flight graph at $t = 15$ ms in $x - y$ plane for the condensate at overcritical rotation ($\Omega/\omega_\perp = 1.05$). $T = 50$ nK $< T_c = 55.5$ nK ($\beta = 6.2 \times 10^{-2}$). The linear size of the profile is 67 μm.

Time-of-flight graphs for BECs (13)



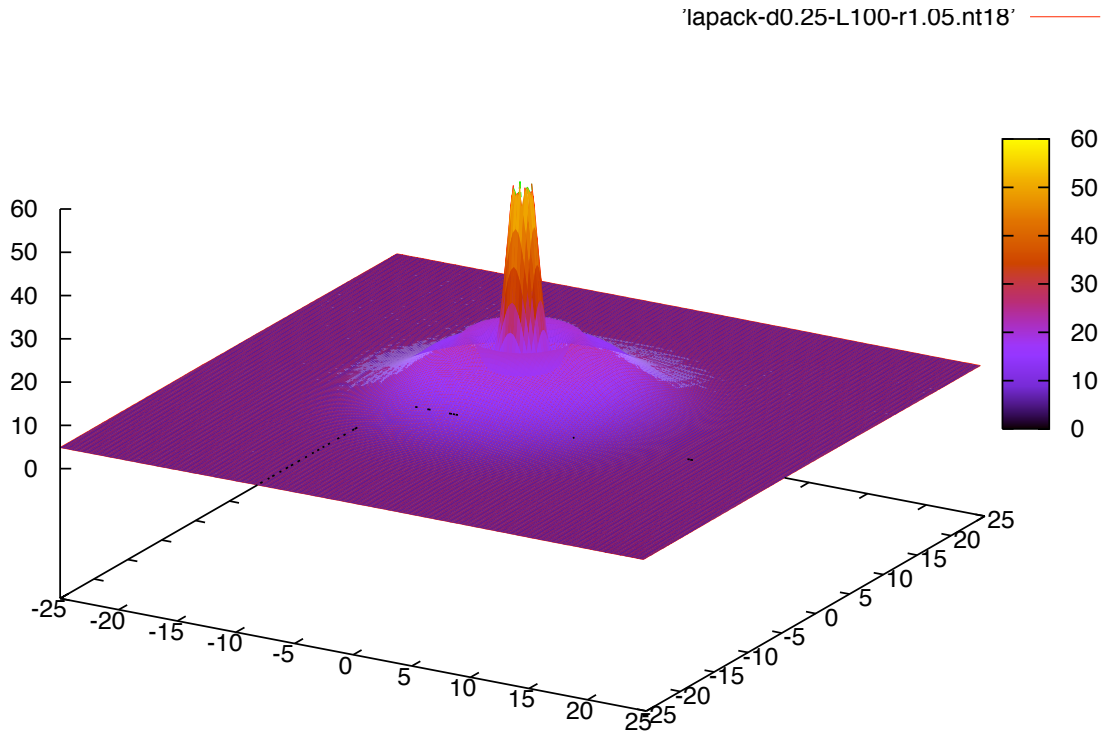
Time-of-flight graph at $t = 16$ ms in $x - y$ plane for the condensate at overcritical rotation ($\Omega/\omega_\perp = 1.05$). $T = 50$ nK $< T_c = 55.5$ nK ($\beta = 6.2 \times 10^{-2}$). The linear size of the profile is 67 μm.

Time-of-flight graphs for BECs (14)



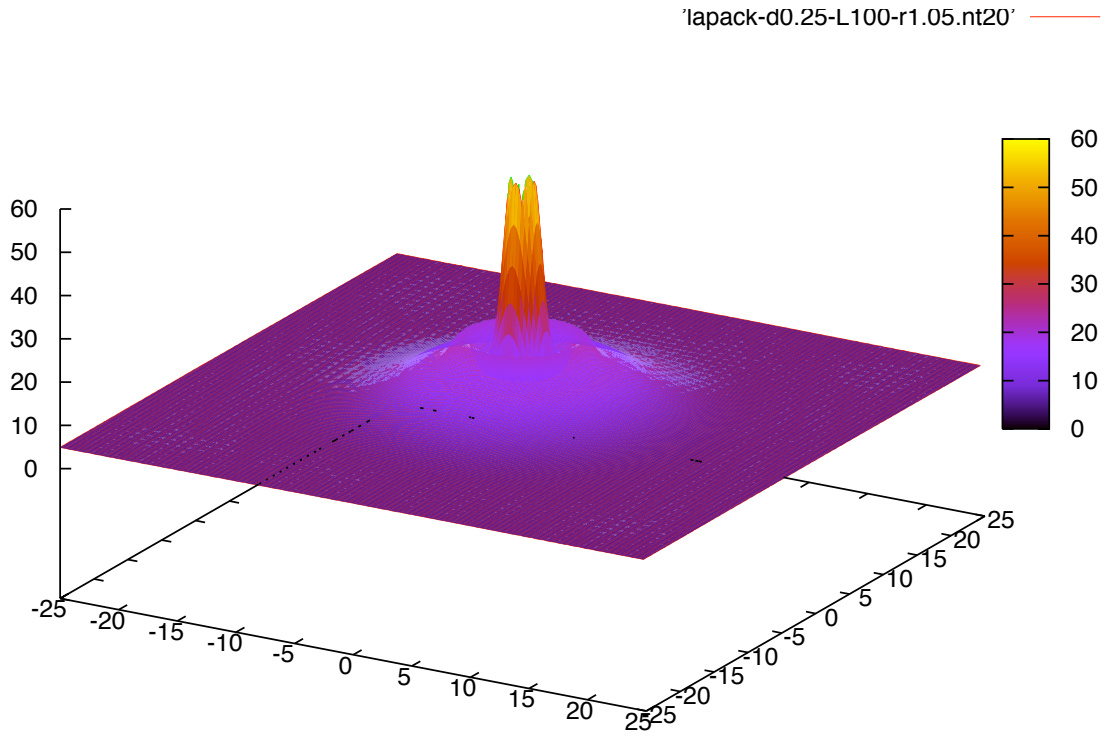
Time-of-flight graph at $t = 17$ ms in $x - y$ plane for the condensate at overcritical rotation ($\Omega/\omega_\perp = 1.05$). $T = 50$ nK $< T_c = 55.5$ nK ($\beta = 6.2 \times 10^{-2}$). The linear size of the profile is 67 μm.

Time-of-flight graphs for BECs (15)



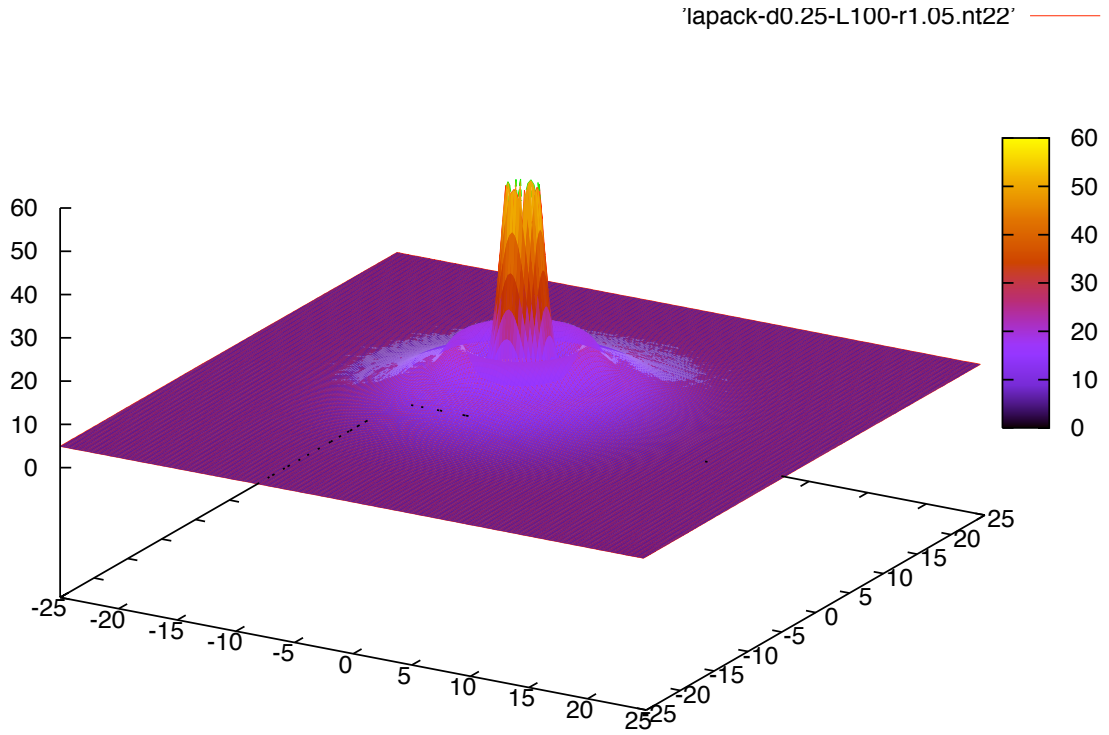
Time-of-flight graph at $t = 18$ ms in $x - y$ plane for the condensate at overcritical rotation ($\Omega/\omega_\perp = 1.05$). $T = 50$ nK $< T_c = 55.5$ nK ($\beta = 6.2 \times 10^{-2}$). The linear size of the profile is 67 μm.

Time-of-flight graphs for BECs (16)



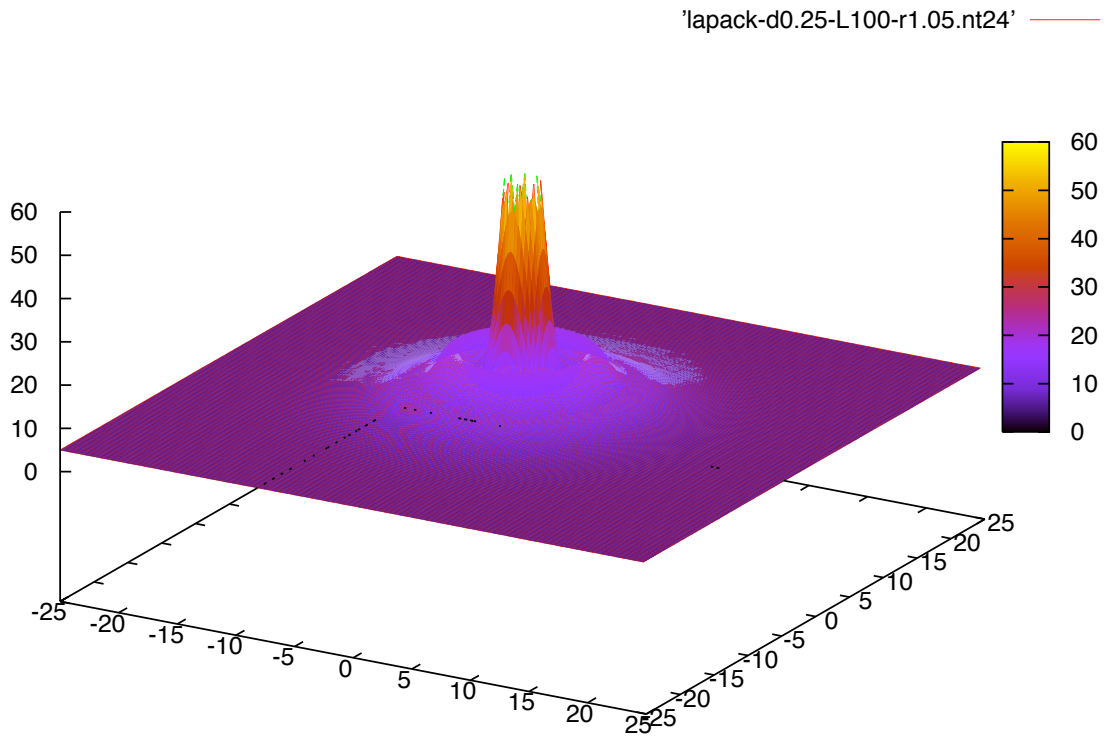
Time-of-flight graph at $t = 20$ ms in $x - y$ plane for the condensate at overcritical rotation ($\Omega/\omega_\perp = 1.05$). $T = 50$ nK $< T_c = 55.5$ nK ($\beta = 6.2 \times 10^{-2}$). The linear size of the profile is 67 μm.

Time-of-flight graphs for BECs (17)



Time-of-flight graph at $t = 22$ ms in $x - y$ plane for the condensate at overcritical rotation ($\Omega/\omega_\perp = 1.05$). $T = 50$ nK $< T_c = 55.5$ nK ($\beta = 6.2 \times 10^{-2}$). The linear size of the profile is 67 μm.

Time-of-flight graphs for BECs (18)



Time-of-flight graph at $t = 24$ ms in $x - y$ plane for the condensate at overcritical rotation ($\Omega/\omega_\perp = 1.05$). $T = 50$ nK $< T_c = 55.5$ nK ($\beta = 6.2 \times 10^{-2}$). The linear size of the profile is 67 μm.

Conclusions (1)

- We have presented a new method for numerical calculation of path integrals for a general non-relativistic many-body quantum theory
- We have derived discretized effective actions which allow deeper analytical understanding of the path integral formalism
  - Gaussian halving
  - ϵ-expansion of the short-time propagator
  - recursive approach
- In the numerical approach, discretized effective actions of level p provide substantial speedup of Monte Carlo algorithm from $1/N$ to $1/N^p$
- For single-particle one-dimensional theories we have derived discretized actions up to level $p = 35$, while for a general non-relativistic many-body theory up to level $p = 10$

Conclusions (2)

- For special cases of potentials we have derived effective actions to higher levels ($p = 140$ for a quartic anharmonic oscillator in $d = 1$, $p = 67$ in $d = 2$, $p = 37$ for modified Pöschl-Teller potential)
- We have developed MC codes that implement the newly introduced approached, as well as *Mathematica* codes for automation of symbolic derivation of discretized effective actions for higher values of level p
- The derived effective actions are used for the numerical study of properties of (fast-rotating) ideal Bose-Einstein condensates
  - Eigenvalues and eigenstates
  - Condensation temperature and ground-state occupancy
  - Density profiles and time-of-flight graphs

Further applications

- Ground states of low-dimensional quantum systems
- Properties of interacting Bose-Einstein condensates
  - Gross-Pitaevskii (mean field) equation
  - Effective actions for time-dependent potentials
- Quantum gases with disorder (Anderson localization)
- Improved estimators for expectations values (heat capacity, magnetization etc.)

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- Ivana Vidanović
- Danica Stojiljković
- Jelena Grujić
- dr Axel Pelster

Effective discretized p=4 action

$$
\begin{aligned}
S_N^{(p=4)} &= \sum \left\{ \epsilon \left(\frac{1}{2} \frac{\delta_i \delta_i}{\epsilon^2} + V \right) \right. \\
&+ \frac{\epsilon^2}{12} \partial^2_{k,k} V + \frac{\epsilon \delta_i \delta_j}{24} \partial^2_{i,j} V \\
&- \frac{\epsilon^3}{24} \partial_i V \partial_i V + \frac{\epsilon^3}{240} \partial^4_{i,i,j,j} V + \frac{\epsilon^2 \delta_i \delta_j}{480} \partial^4_{i,j,k,k} V + \frac{\epsilon \delta_i \delta_j \delta_k \delta_l}{1920} \partial^4_{i,j,k,l} V \\
&+ \frac{\epsilon^4}{6720} \partial^6_{i,i,j,j,k,k} V - \frac{\epsilon^4}{120} \partial_i V \partial^3_{i,k,k} V - \frac{\epsilon^4}{360} \partial^2_{i,j} V \partial^2_{i,j} V \\
&- \frac{\epsilon^3 \delta_i \delta_j}{480} \partial_k V \partial^3_{k,i,j} V + \frac{\epsilon^3 \delta_i \delta_j}{13440} \partial^6_{i,j,k,k,l,l} V - \frac{\epsilon^3 \delta_i \delta_j}{1440} \partial^2_{i,k} V \partial^2_{k,j} V \\
&+ \left. \frac{\epsilon^2 \delta_i \delta_j \delta_k \delta_l}{53760} \partial^6_{i,j,k,l,m,m} V + \frac{\epsilon \delta_i \delta_j \delta_k \delta_l \delta_m \delta_n}{322560} \partial^6_{i,j,k,l,m,n} V \right\}
\end{aligned}
$$