Path Integrals Without Integrals

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Overview

- Introduction
  - Path integral formalism
  - Discretized effective actions
  - Ideal discretization
- Recursive approach
  - Improving effective actions
  - Recursive relations
  - Numerical verification
  - Effective actions
- Application to BECs
  - Path integrals without integrals
  - Thermodynamic properties
  - Density profiles and time-of-flight graphs
- Concluding remarks

Path integral formalism (1)

- Amplitudes for transition from an initial state $|\alpha\rangle$ to a final state $|\beta\rangle$ in imaginary time T can be written as

$$A(\alpha,\beta;T) = \langle\beta|e^{-T\hat{H}}|\alpha\rangle$$

- Dividing the evolution into N time steps $\epsilon = T/N$, we get

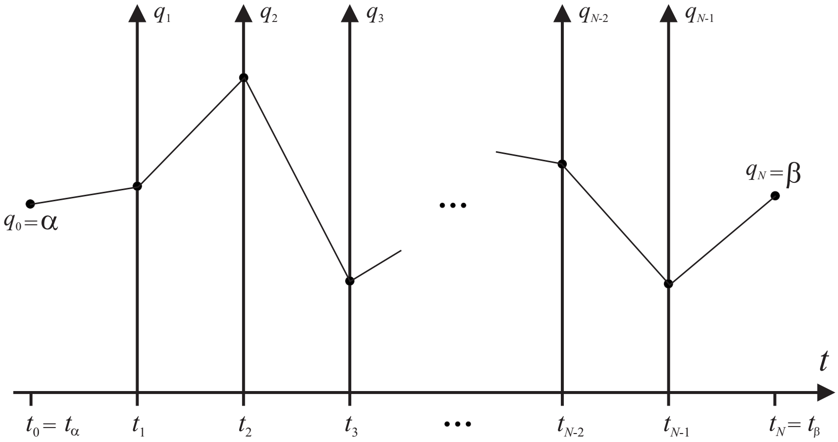
$$A(\alpha,\beta;T) = \int dq_1 \cdots dq_{N-1} A(\alpha,q_1;\epsilon) \cdots A(q_{N-1},\beta;\epsilon)\,,$$

- Approximate calculation of short-time amplitudes leads to

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

- Hagen Kleinert, *Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets*, 5$^{\text{th}}$ edition, World Scientific, Singapore, 2009.

Path integral formalism (2)



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

Discretized effective actions

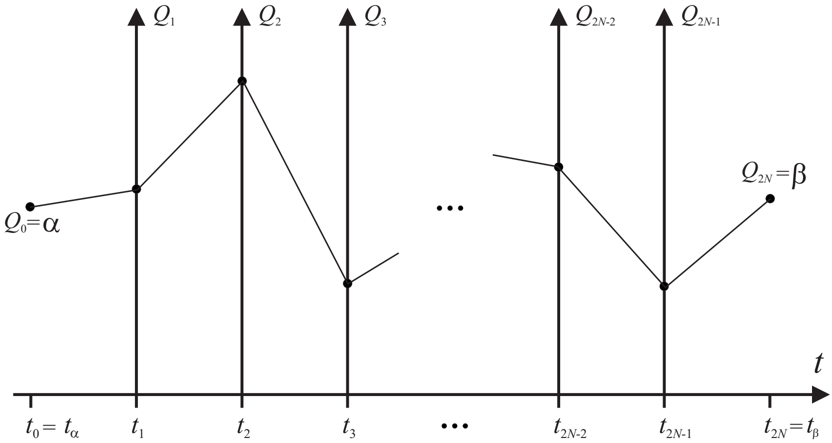
- Discretized actions can be classified according to the speed of convergence of discretized path integrals
- Improved discretized actions have been earlier constructed, mainly tailored for calculation of partition functions
    - generalizations of the Trotter-Suzuki formula
    - improvements in the short-time propagation
    - expansion of the propagator by the number of derivatives
- Li-Broughton effective potential (1987)

$$V^{LB} = V + \frac{1}{24}\epsilon^2 \left(\nabla V\right)^2$$

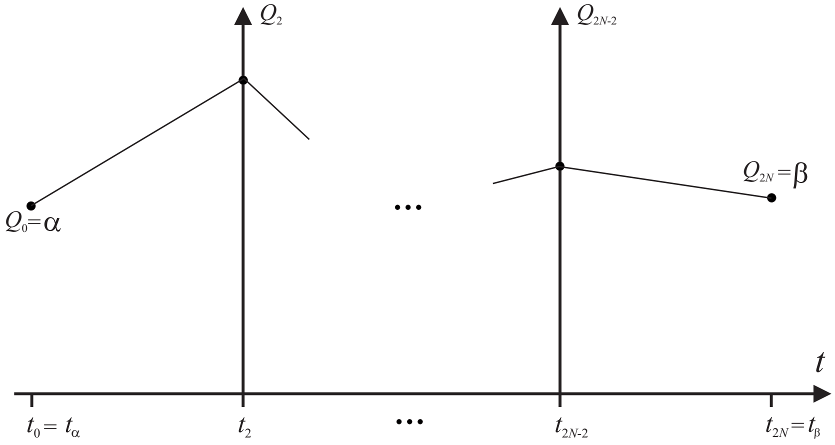
in the left prescription gives $1/N^4$ convergence for Z

- This cannot be extended to higher orders, nor such an approach was developed for general transition amplitudes
- Initial, RG-based approach: Gaussian halving

Gaussian halving (1)



Gaussian halving (2)



Ideal discretization

- Ideal discretized action S^* is defined as the action giving exact continual amplitudes $A_N = A$ for any discretization
- 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 short-time discretized action S_n^* is given by

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

where M is the number of particles, d dimensionality, and

$$S_n^* = \frac{\delta_n^2}{2\epsilon} + \epsilon W_n(\bar{q}_n, \delta_n; \epsilon)\,,$$

and W is the (ideal) effective potential

Improving effective actions (1)

- We start from Schrödinger's equation for the short-time amplitude $A(q,q';\epsilon)$

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

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

- 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.

Improving effective actions (2)

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

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

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 (1)

- The effective potential is given as a power series

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

where systematics in ϵ-expansion is ensured by $\epsilon \propto x^2$, and

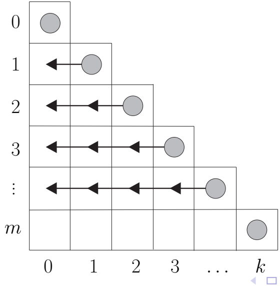
$$W_{m,k}(x,\bar{x})=x_{i_1}x_{i_2}\cdots x_{i_{2k}}c_{m,k}^{i_1,\ldots,i_{2k}}(\bar{x})$$

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

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

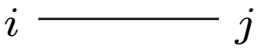
Recursive relations (2)

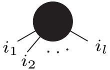
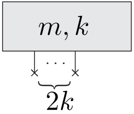
- Diagonal coefficients are easily obtained from recursive relations
$$W_{m,m} = \frac{1}{(2m+1)!}(x \cdot \bar{\partial})^{2m} V$$
- Off-diagonal coefficients are obtained by applying recursive relations in the following order



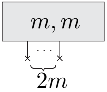
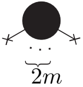
Diagrammatic form of effective actions (1)

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

$\delta_{ij} =$  , $x_i =$ 

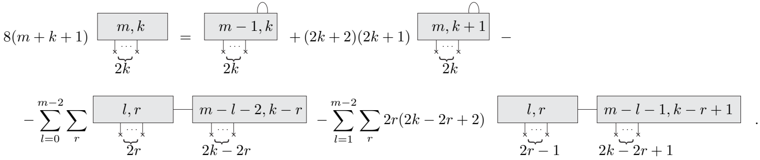
$\bar{\partial}_{i_1} \bar{\partial}_{i_2} \cdots \bar{\partial}_{i_l} V =$  , $W_{m,k} =$  .

- Diagrammatic form of diagonal coefficients

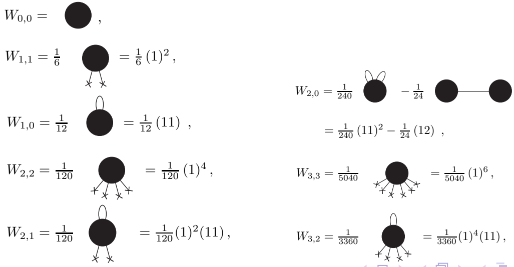
$W_{m,m} =$  $= \frac{1}{(2m+1)!}$  .

Diagrammatic form of effective actions (2)

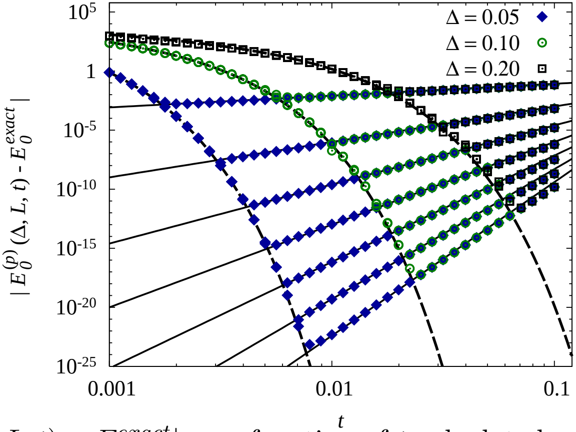
- Diagrammatic form of recursive relations



- Solutions to level $p = 3$

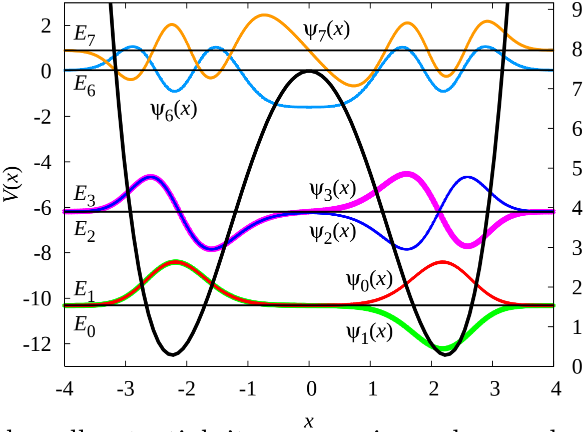


Diagonalization of the evolution operator



$|E_0^{(p)}(\Delta, L, t) - E_0^{exact}|$ as a function of t calculated using level $p = 1, 3, 5, 7, 9, 11, 13$ effective action for the quartic anharmonic potential, with $m = \omega = 1$, $g = 48$, $\Delta = 0.05$, $L = 4$.

Energy eigenvalues and eigenstates



The double-well potential, its energy eigenvalues and eigenfunctions $\psi_k(x)$ for $k = 0, 1, 2, 3, 6, 7$, with the parameters $m = -10$, $\omega = 1$, $g = 12$, $L = 10$, $\Delta = 1.22 \cdot 10^{-3}$, $t = 0.1$.

Effective actions: many-body p=4 result

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

Effective actions: time-dependent formalism

$$W(\mathbf{x},\bar{\mathbf{x}};\varepsilon,\tau)=\sum_{m=0}^{\infty}\sum_{k=0}^{m}\left\{W_{m,k}(\mathbf{x},\bar{\mathbf{x}};\tau)\,\varepsilon^{m-k}+W_{m+1/2,k}(\mathbf{x},\bar{\mathbf{x}};\tau)\,\varepsilon^{m-k}\right\},$$

$$\mathbf{R1}:8(m+k+1)\,W_{m,k}=8\frac{\Pi(m,k)\,(\bar{\mathbf{x}}\cdot\boldsymbol{\partial})^{2k}\overset{(m-k)}{V}}{(2k)!\,(m-k)!\,2^{m-k}}+\bar{\partial}^2\,W_{m,k+1}+\partial^2\,W_{m-1,k}$$
$$-\sum_{l,r}\left\{\boldsymbol{\partial}W_{l,r}\cdot\boldsymbol{\partial}W_{m-l-2,k-r}+\boldsymbol{\partial}W_{l+1/2,r}\cdot\boldsymbol{\partial}W_{m-l-5/2,k-r-1}\right.$$
$$\left.+\bar{\boldsymbol{\partial}}W_{l,r}\cdot\bar{\boldsymbol{\partial}}W_{m-l-1,k-r+1}+\bar{\boldsymbol{\partial}}W_{l+1/2,r}\cdot\bar{\boldsymbol{\partial}}W_{m-l-3/2,k-r}\right\},$$

$$\mathbf{R2}:8(m+k+2)\,W_{m+1/2,k}=8\frac{(1-\Pi(m,k))\,(\bar{\mathbf{x}}\cdot\boldsymbol{\partial})^{2k+1}\overset{(m-k)}{V}}{(2k+1)!\,(m-k)!\,2^{m-k}}+\bar{\partial}^2\,W_{m+1/2,k+1}$$
$$+\partial^2\,W_{m-1/2,k}-\sum_{l,r}\left\{\boldsymbol{\partial}W_{l,r}\cdot\boldsymbol{\partial}W_{m-l-3/2,k-r}+\boldsymbol{\partial}W_{l+1/2,r}\cdot\boldsymbol{\partial}W_{m-l-2,k-r}\right.$$
$$\left.+\bar{\boldsymbol{\partial}}W_{l+1/2,r}\cdot\bar{\boldsymbol{\partial}}W_{m-l-1,k-r+1}+\bar{\boldsymbol{\partial}}W_{l,r}\cdot\bar{\boldsymbol{\partial}}W_{m-l-1/2,k-r+1}\right\}.$$

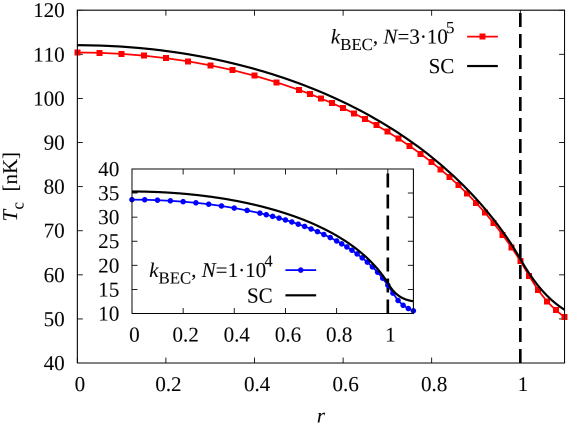
Rotating ideal Bose gases

- 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)]

Path integrals without integrals

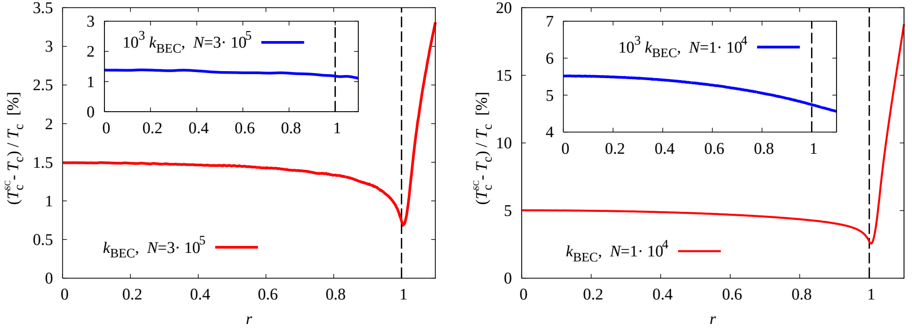
- Using the large number of energy eigenvalues and eigenvectors of one-particle states, calculated by the exact diagonalization of the evolution operator, we study global and local properties of condensates
- $V_{BEC} = \frac{M}{2}(\omega_\perp^2 - \Omega^2)r_\perp^2 + \frac{M}{2}\omega_z^2 z^2 + \frac{k_{\rm BEC}}{4} r_\perp^4$, $\omega_\perp = 2\pi \times 64.8$ Hz, $\omega_z = 2\pi \times 11.0$ Hz, $k_{\rm BEC} = 2.6 \times 10^{-11}$ Jm^{-4}
- Typical values of the dimensionless inverse temperature $\beta_{\rm eff} = \hbar\omega_\perp / k_{\rm B} T \lesssim 0.1$ represent already short (imaginary) times of propagation
- Hence, one-time-step (analytic) approximation to the calculation of BEC properties in the path integral formalism can be applied

Condensation temperature (1)



T_c of a condensate in an anharmonic trap for different rotation frequencies $r = \Omega/\omega_\perp$, obtained with $p = 21$ effective action. SC calculation: S. Kling and A. Pelster, PRA **76**, 023609 (2007).

Condensation temperature (2)



Relative error of SC approximation for T_c of a condensate in an anharmonic trap for different rotation frequencies $r = \Omega/\omega_\perp$. Numerical results are obtained with $p = 21$ effective action.

Density profiles and time-of-flight graphs (1)

- Density profile is given in terms of the diagonal two-point propagator $n(\mathbf{r}) = \rho(\mathbf{r}, \mathbf{r}) = \langle \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}(\mathbf{r}) \rangle$, and for the ideal Bose gas

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

- 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)

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

where

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

Density profiles and time-of-flight graphs (2)

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Evolution of the $x - y$ density profile of over-critically rotating ($\Omega/\omega_\perp = 1.05$) condensate at $T = 10$ nK $< T_c = 55.3$ nK. The linear size of the profile is 54 μm.

Conclusions

- New method for numerical calculation of path integrals for a general non-relativistic many-body quantum theory
- In the numerical approach, discretized effective actions of level p provide substantial speedup of Monte Carlo algorithm from $1/N$ to $1/N^p$
- If the time of propagation/inverse temperature is small, analytic one-time-step approximation can be used: path integrals without integrals
- The derived results used to study properties of quantum systems by numerical diagonalization of the space-discretized evolution operator
- Numerical study of properties of (fast-rotating) ideal Bose-Einstein condensates
    - Condensation temperature and ground-state occupancy
    - Density profiles and time-of-flight graphs

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- Mathematica and PIMC codes: http://www.scl.rs/speedup/

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