Recursive Approach to the Calculation of Improved Effective Actions

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Overview

- Effective actions
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  - Discretized effective actions
  - Recursive approach
  - Effective action for many-body systems
- Exact diagonalization of the evolution operator
  - Discretization approach
  - Space-discretization errors
  - Evolution-time errors
  - Energy eigenvalues and eigenstates
- Application to BECs
  - Rotating ideal Bose gases
  - Calculation of global properties
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- Concluding remarks

Formulation of the path integral formalism (1)

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

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

- For technical reasons, usually we use imaginary time
- The standard derivation starts from the identity

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

dividing the evolution into N steps of the length $\epsilon = T/N$. This expression is exact.

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

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

Formulation of the path integral formalism (2)

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

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)

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 makes use of the cyclic property of the trace - the improvement is valid for partition functions only

Ideal discretization (1)

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

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

- 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

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

Improving effective actions (1)

- We present an approach enabling a substantial speedup in the convergence of path integrals
- Previously we have set up an approach based on the integral equation connecting discretized effective actions of different coarseness
- It allows the systematic derivation of effective actions and leadis to improved $1/N^p$ convergence for one-particle systems in $d = 1$ - Gaussian halving
- For many-body systems in arbitrary dimensions we have developed two equivalent approaches

Improving effective actions (2)

- 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.
- The presented results are highly related to recently developed systematic approach by Chin and collaborators for the arbitrary-order splitting of the evolution operator

Equation for the ideal effective potential (1)

- 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 (2)

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

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

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)

- 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

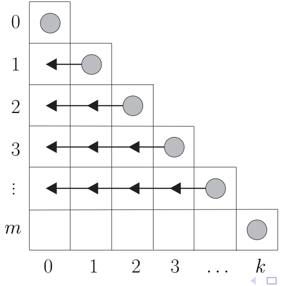
$$\begin{aligned}8\,(m+k+1)\,W_{m,k}&=\bar{\partial}^2W_{m-1,k}+\partial^2W_{m,k+1}-\\&-\sum_{l=0}^{m-2}\sum_{r}(\bar{\partial}W_{l,r})\cdot(\bar{\partial}W_{m-l-2,k-r})-\\&-\sum_{l=1}^{m-2}\sum_{r}(\partial W_{l,r})\cdot(\partial W_{m-l-1,k-r+1})\end{aligned}$$

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 action for many-body systems (1)

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

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

Effective action for many-body systems (2)

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

Space-discretized Hamiltonian (1)

- Coordinate representation of the time-independent Schrödinger's equation

$$\int \mathrm{d}y \, \langle x|\hat{H}|y\rangle \, \langle y|\psi\rangle = E \, \langle x|\psi\rangle$$

- Numerical implementation of the exact diagonalization: continuous coordinates x replaced by a discrete space grid $x_n = n\Delta$
- To represent this on a computer, we still have to restrict the integers n to a finite range, which is equivalent to introducing a space cutoff L, or putting the system in a infinitely high potential box

Space-discretized Hamiltonian (2)

- For example, the rectangular quadrature rule leads to the following space-discretized Schrödinger equation

$$\sum_{m=-N}^{N-1} H_{nm} \langle m\Delta|\psi\rangle = E(\Delta, L)\, \langle n\Delta|\psi\rangle\,,$$

  where $H_{nm} = \Delta \cdot \langle n\Delta|\hat{H}|m\Delta\rangle$, $N = [L/\Delta]$
- As a result, we have obtained a $2N \times 2N$ matrix that represents the Hamiltonian of the system
- The eigenvalues of this matrix depend on the two parameters introduced in the above discretization process: cutoff L and discretization step Δ
- Continuous physical quantities are recovered in the limit $L \to \infty$ and $\Delta \to 0$

Space-discretized Hamiltonian (3)

- The two approximations (Δ, L) involved in the discretization procedure are common steps in solving eigenproblems of Hamiltonians
- The system is effectively surrounded by an infinitely high wall, and as the cutoff L tends to infinity, we approach the exact energy levels always from above, which is a typical variational behavior
- The effects of the discretization step Δ are much more complex, and follow from the fact that the kinetic energy operator cannot be exactly represented on finite real-space grids

Space-discretized evolution operator

- Here we instead use the approach of diagonalization of the space-discretized evolution operator, introduced first by Sethia et al. [J. Chem. Phys. **93** (1990) 7268]

$$\sum_{m=-N}^{N-1} A_{nm}(t)\,\langle m\Delta|\psi\rangle = e^{-t\,E(\Delta,L,t)}\,\langle n\Delta|\psi\rangle\,,$$

where $A_{nm}(t) = \Delta \cdot A(n\Delta, m\Delta; t) = \Delta \cdot \langle n\Delta|e^{-t\hat{H}}|m\Delta\rangle$

- In this approach the time of evolution t plays the role of an auxiliary parameter which is not related to the discretization, but numerically calculated eigenvalues and eigenstates will necessarily depend on it
- We also carefully study the errors associated with the discretization and numerical diagonalization

Errors due to the spacing Δ (1)

- Using the Poisson summation formula we find that the space discretized free-particle amplitude satisfies

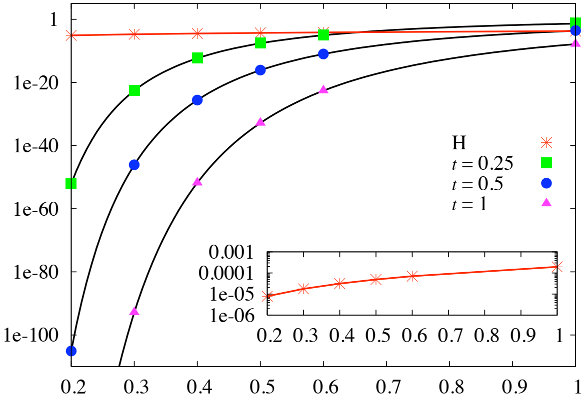
$$\sum_{n\in\mathbb{Z}} A_{nm}(t) = \sum_{n\in\mathbb{Z}} e^{-\frac{2\pi^2}{\Delta^2}n^2 t} \approx 1 + 2\exp\left(-\frac{2\pi^2}{\Delta^2}t\right)$$

- This leads to discretization errors for energy eigenvalues

$$E_k(\Delta, L, t) - E_k \sim -\frac{1}{t}\,\exp\left(-\frac{2\pi^2}{\Delta^2}t\right)$$

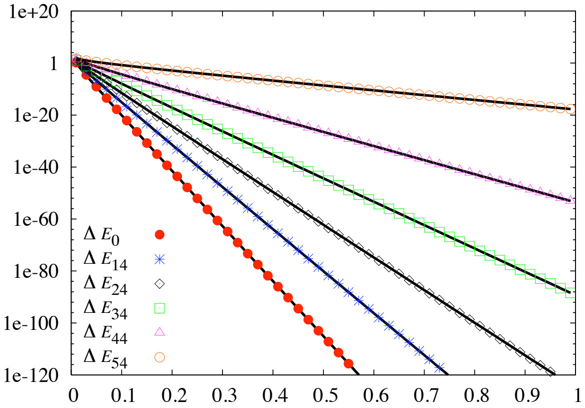
- Note that the effect of discretization is non-perturbative in discretization step Δ, i.e. it is smaller than any power of Δ

Errors due to the spacing Δ (2)



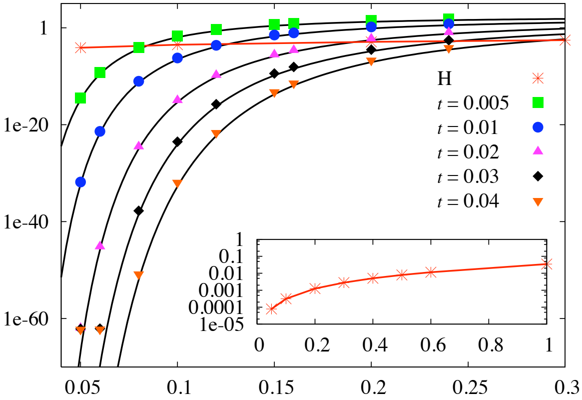
$|E_0(\Delta, L, t) - E_0|$ for a free particle in a box as a function of Δ for different values of time of evolution t and $L = 6$.

Errors due to the spacing Δ (3)



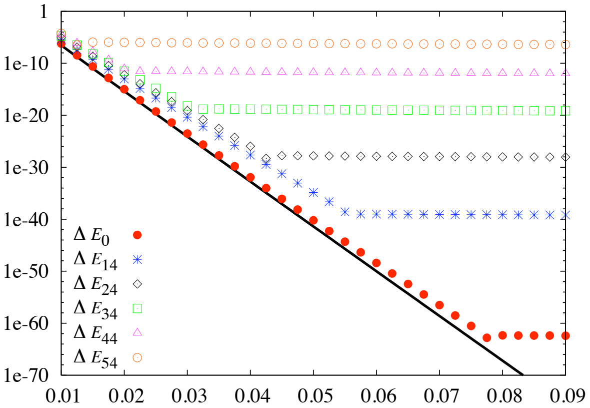
$|E_k(\Delta, L, t) - E_k|$ for a free particle in a box as a function of t for several energy levels k. The parameters used are $L = 6$, $\Delta = 0.2$.

Errors due to the spacing Δ (4)



$|E_0(\Delta, L, t) - E_0|$ for a harmonic oscillator as a function of Δ for different values of time of evolution t, with $L = 12$, $\omega = 1$, $M = 1$.

Errors due to the spacing Δ (5)



$|E_k(\Delta, L, t) - E_k|$ for a harmonic oscillator as a function of t for several energy levels k. The parameters used are $L = 12$, $\Delta = 0.1$, $\omega = 1$, $M = 1$.

Errors due to the space-cutoff L (1)

- The effects of space cutoffs are known for continuous-space theories. The shift in energy level $E_k(L) - E_k$ is found to be positive

$$E_k(L) - E_k = C_k(a) \left(\int_a^L \frac{\mathrm{d}x}{|\psi_k(x)|^2} \right)^{-1} ,$$

where a is larger than and well away from the largest zero of $\psi_k(x)$, but smaller than and well away from the space cutoff L

- The constant $C_k(a)$ depends on the normalization of eigenfunction and the choice of parameter a. For the ground state we can always choose $a = 0$, so that

$$C_0(0) = \left(\int_{-L}^L \mathrm{d}x \, |\psi_0(x)|^2 \right)^{-1}$$

Errors due to the space-cutoff L (2)

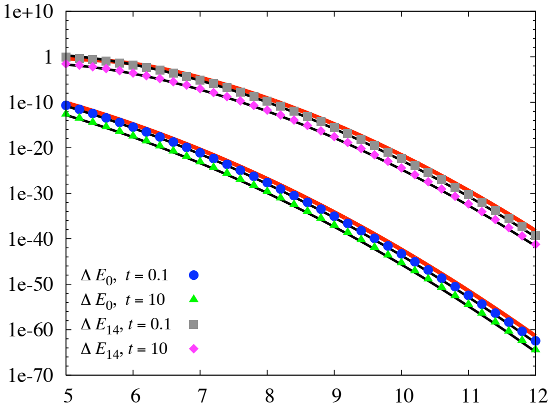
- When we use diagonalization of the discretized amplitudes, the errors in energy level will necessarily also depend on the parameter t and other discretization parameters
- A simple estimate of ground energy errors follows from the spectral decomposition of diagonal amplitudes
- For large t we have $A(x, x; t) \approx |\psi_0(x)|^2 e^{-E_0 t}$. Integrating this we find an approximate result for E_0 for a system with cutoff L

$$E_0(L, t) \approx -\frac{1}{t} \ln \int_{-L}^{L} \mathrm{d}x\, A(x, x; t)$$

In the $L \to \infty$ limit we recover the exact ground energy, so that a simple estimate of finite size effects on E_0 is given by

$$E_0(L, t) - E_0 \approx \frac{1}{t} \int_{|x|>L} \mathrm{d}x\, |\psi_0(x)|^2$$

Errors due to the space-cutoff L (3)



$E_k(\Delta, L, t) - E_k$ for a harmonic oscillator as a function of space cutoff L for different values of time of evolution t, with $\Delta = 0.1$, $\omega = 1$, $M = 1$.

Evolution-time errors (1)

- The precise calculation of transition amplitudes is essential for applications of this method
- In papers by Sethia et al. all calculations are based on the naive approximation for amplitudes

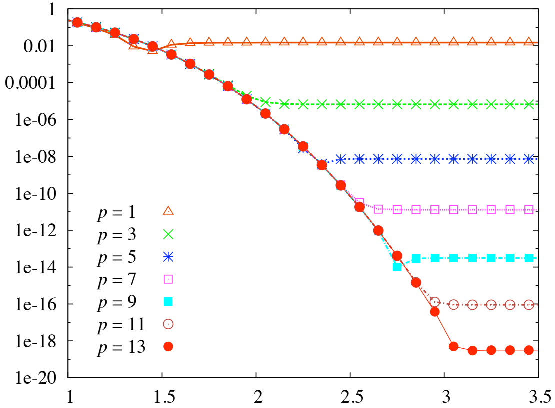
$$A^{(1)}(x,y;t) \approx \frac{1}{(2\pi t)^{d/2}}\, e^{-\frac{(x-y)^2}{2t} - tV\left(\frac{x+y}{2}\right)}$$

- We use effective action approach, which gives closed-form analytic expressions $A^{(p)}(x,y;t)$ for short-time transition amplitudes,

$$A^{(p)}(x,y;t) = A(x,y;t) + O(t^p)$$

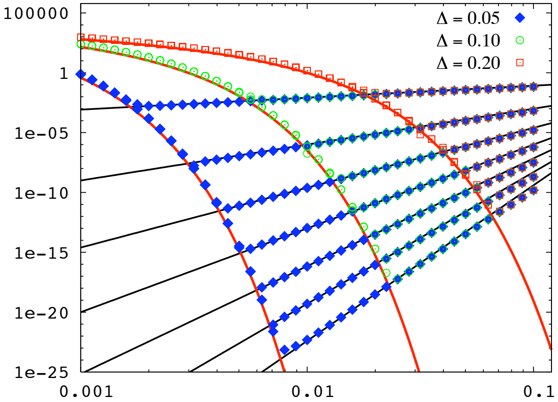
- If p is high enough and time of evolution is less than the radius of convergence of the ϵ-expansion, errors in calculated transition amplitudes are negligible

Evolution-time errors (2)



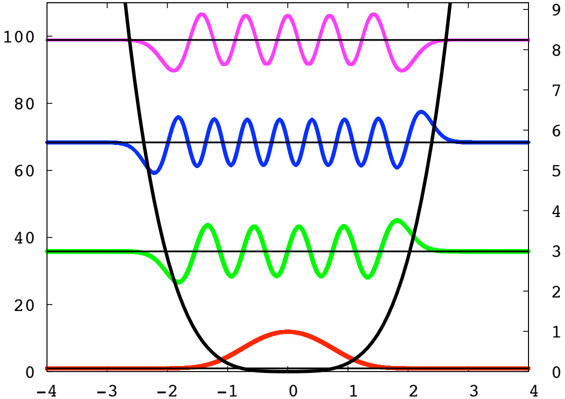
$|E_0^{(p)}(\Delta, L, t) - E_0^{exact}|$ as a function of L calculated using level $p = 1, 3, 5, 7, 9, 11, 13$ effective action for the quartic anharmonic potential, with $M = \omega = 1$, $g/24 = 2$, $\Delta = 0.05$, $t = 0.02$.

Evolution-time errors (3)



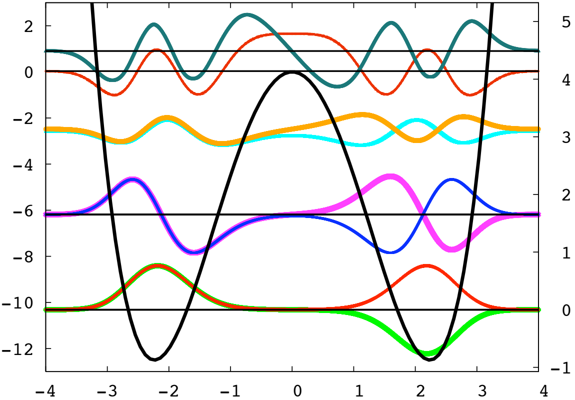
$|E_0^{(p)}(\Delta, L, t) - E_0^{exact}|$ as a function of t calculated using level $p = 1, 3, 5, 7, 9, 11, 13$ effective action for the quartic anharmonic potential, with $M = \omega = 1$, $g/24 = 2$, $\Delta = 0.05$, $L = 4$.

Energy eigenvalues and eigenstates in $d = 1$ (1)



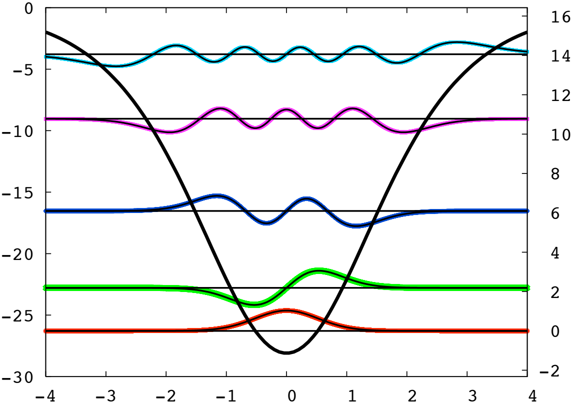
The quartic anharmonic potential, its energy eigenvalues (horizontal lines) and eigenfunctions $\psi_k(x)$ for $k = 0, 9, 15, 20$, with the parameters $p = 21$, $M = \omega = 1$, $g = 48$, $L = 8$, $\Delta = 9.76 \cdot 10^{-4}$, $t = 0.02$.

Energy eigenvalues and eigenstates in $d = 1$ (2)



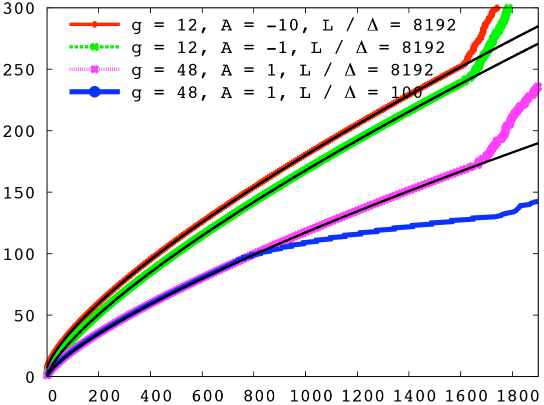
The double-well potential, its energy eigenvalues (horizontal lines) and eigenfunctions $\psi_k(x)$ for $k = 0, 1, 2, 3, 4, 5, 6, 7$, with the parameters $M = -10$, $\omega = 1$, $g = 12$, $L = 10$, $\Delta = 1.22 \cdot 10^{-3}$, $t = 0.1$.

Energy eigenvalues and eigenstates in $d = 1$ (3)



The modified Pöschl-Teller potential, its energy eigenvalues (horizontal lines) and eigenfunctions $\psi_k(x)$ for $k = 0, 1, 3, 6, 9$, with the parameters $\alpha = 0.5$, $\lambda = 15.5$, $p = 21$, $L = 8$, $\Delta = 9.76 \cdot 10^{-4}$, $t = 10^{-3}$.

Energy eigenvalues and eigenstates in $d = 1$ (4)



Cumulative distribution of the density of numerically obtained energy eigenstates for the quartic anharmonic and double-well potential, for $\omega = 1$ and the following values of diagonalization parameters: $p = 21$, $L = 10$ for $M = -10, -1$ and $L = 8$ for

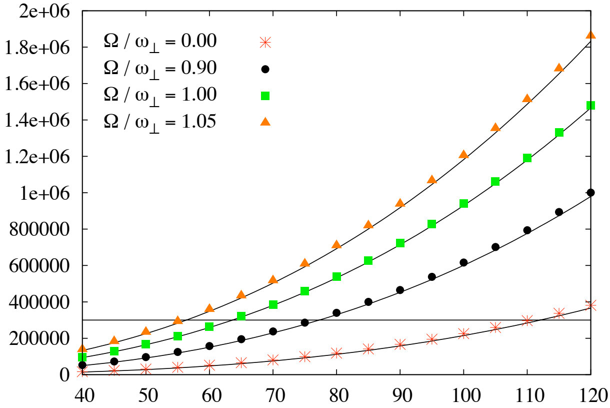
Rotating ideal Bose gases (1)

- 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)]

Rotating ideal Bose gases (2)

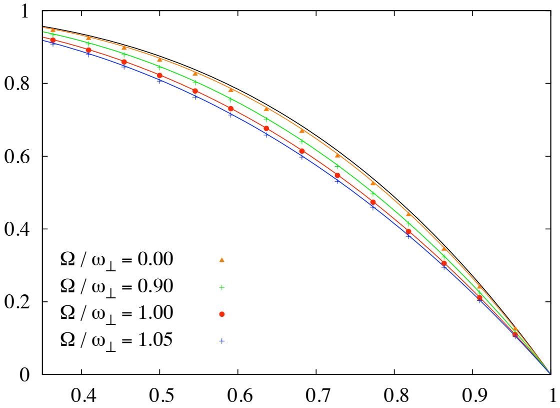
- We apply the developed discretized effective approach to the study of properties of such (fast-rotating) Bose-Einstein condensates
- We calculate large number of energy eigenvalues and eigenvectors of one-particle states
- We numerically study global properties of the condensate
  - T_c as a function of rotation frequency Ω
  - ground state occupancy N_0/N as a function of temperature
- We calculate density 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}

Condensation temperature



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

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 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 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

$$n(\vec{r},t) = N_0|\psi_0(\vec{r},t)|^2 + \sum_{m\geq 1}\Bigg[e^{m\beta E_0}\int \frac{\mathrm{d}^3\vec{k}_1\,\mathrm{d}^3\vec{k}_2\,\mathrm{d}^3\vec{R}_1\,\mathrm{d}^3\vec{R}_2}{(2\pi)^6}\times$$

$$e^{-i(\omega_{\vec{k}_1}-\omega_{\vec{k}_2})t+i(\vec{k}_1-\vec{k}_2)\cdot\vec{r}-i\vec{k}_1\cdot\vec{R}_1+i\vec{k}_2\cdot\vec{R}_2}\,A(\vec{R}_1,0;\vec{R}_2,m\beta\hbar) - |\psi_0(\vec{r},t)|^2\Bigg]$$

- 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)

(Loading diag-d025-L400-r09eps02beta0311.mpg)

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 (4)

(Loading diag-d025-L400-r10eps02beta0311.mpg)

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 (5)

(Loading diag-d025-L400-r105eps02beta0311.mpg)

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.

Conclusions (1)

- New method for numerical calculation of path integrals for a general non-relativistic many-body quantum theory
- Derived discretized effective actions allow deeper analytical understanding of the path integral formalism
- 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 approaches, as well as *Mathematica* codes for automation of symbolic derivation of discretized effective actions
- 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

Further applications

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

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References

- A. Bogojević, A. Balaž, A. Belić, PRL **94**, 180403 (2005)
- A. Bogojević, A. Balaž, A. Belić, PLA **344**, 84 (2005)
- A. Bogojević, A. Balaž, A. Belić, PRB **72**, 064302 (2005)
- A. Bogojević, A. Balaž, A. Belić, PRE **72**, 036128 (2005)
- D. Stojiljković, A. Bogojević, A. Balaž, PLA **360**, 205 (2006)
- J. Grujić, A. Bogojević, A. Balaž, PLA **360**, 217 (2006)
- A. Bogojević, I. Vidanović, A. Balaž, A. Belić, PLA **372**, 3341 (2008)
- A. Balaž, A. Bogojević, I. Vidanović, A. Pelster, PRE **79**, 036701 (2009)