Path Integrals without Integrals

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Motivation

Path integral Monte Carlo (PIMC) is one of the most important numerical methods for ab initio studies of properties of quantum and statistical physical systems. Here we address an important problem of improving the convergence of PIMC algorithms through the introduction of effective discretized actions. We present an analytic derivation of improved effective actions and apply the N=1 time-slice approximation for the calculation of the critical temperature of a Bose-Einstein condensate of ^{87}Rb atoms in an anharmonic trap.

EFFECTIVE ACTIONS

- Recently, the study of the relationship between discretizations of different coarseness has resulted in the construction of a hierarchy of effective discretized actions $S_N^{(p)}$ with $O(\varepsilon^p)$ convergence [2,3].
- Further, the existence and basic properties of the ideal discretized action S_N^* giving immediately the continuum result $(A_N^* = A)$ were established in [4].
- The effective discretized actions were calculated in [2,3] for the case of one-particle systems as short-time expansions of S_N^* in the form of double series in time ε and in discretized velocities $\delta_n = q_{n+1} - q_n$. This approach was extended to real many-body systems in arbitrary dimensions in [5], and it was shown that the ideal effective action satisfies

$$A(q_n, q_{n+1}; \varepsilon) \propto e^{-S^*} = e^{-\frac{\delta_n^2}{2\varepsilon} - \varepsilon W(\bar{q}_n, \delta_n^2; \varepsilon)},$$

where $\bar{q}_n = \frac{q_n + q_{n+1}}{2}$ is the mid-point.

RECURSIVE RELATIONS

- Starting from the earlier established cummulant ansatz for the short-time amplitude,

$$A(\varepsilon) = A_{FP}(\varepsilon)\ \exp\sum_{n=1}^{\infty}\sum_{k=0}^{n-1} d_{n,k}\varepsilon^{n-k}\delta^{2k},$$

where A_{FP} represents the free massless particle amplitude, the Schrödinger equation for $A(\varepsilon)$ gives a hierarchy of recursive relations for coefficients $d_{n,k}$,

$$\begin{aligned}&(n+k-1)d_{n,k-1} - k(2k-1)d_{n,k} + \frac{\partial V}{4}\partial d_{n-2,k-1}\\ &-\frac{1}{8}\partial^2 d_{n-1,k-1} + \frac{\partial^2 V}{8}\delta_{n,2}\delta_{k,1} - \frac{(\partial V)^2}{8}\delta_{n,3}\delta_{k,1}\\ &+\frac{\partial^{2n-2}V}{(2n-2)!2^{2n-2}}\delta_{n,k} - \sum_{m=2}^{n}\sum_{l=0}^{m-1}\left[2l(k-l)d_{n-m,k-l}d_{m,l}\right.\\ &\left.+\frac{1}{8}\partial d_{n-m-1,k-l-1}\partial d_{m,l}\right] = 0\end{aligned}$$

- The above set of recursive relations can be easily solved to high order in n, i.e. the effective action can be found to high order in ε, since coefficients $d_{n,k}$ are expressed in closed form as functions of previously obtained ones. The initial condition corresponding to the ansatz is $d_{1,0} = 0$.
- This new approach has several important advantages over the older approaches [2-5]:
  - Substantially simpler derivation
  - Much higher values of p accessible
  - Easily generalized to many-particle systems in closed form

EXAMPLE: p=4 ACTION

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

INTRODUCTION

- PIMC calculations start from a quantum-mechanical amplitude $A(a,b;\beta) = \langle b|e^{-\beta H}|a\rangle$ discretized in the form [1] $A_N(a,b;\beta) = \frac{1}{(2\pi\varepsilon)^{N/2}}\int dq_1 \cdots dq_{N-1} e^{-S_N}$, where N is the number of time slices $\varepsilon = \beta/N$, S_N is the discretized action. Using PIMC approach one can also calculate the partition function or various expectation values.
- The use of the naive discretized action yields slow $O(\varepsilon)$ convergence of discretized quantities to continuum limits.
- While the application of various MC methods ensures the optimal dealing with the calculation of multiple integrals, improvements in discretized actions are a well-known problem tackled from several directions in the past, with the aim of speeding up the slow $O(\varepsilon)$ convergence of calculated properties of physical systems.

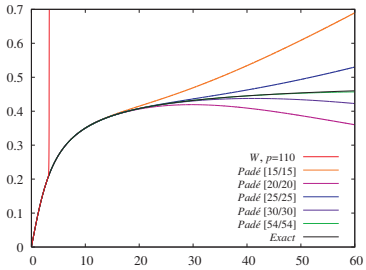

Fig. 1: N=1 effective potential W for $A(0,0,\beta)$ as a function of β for a harmonic oscillator with p=110, its Padé approximants, and the exact result.

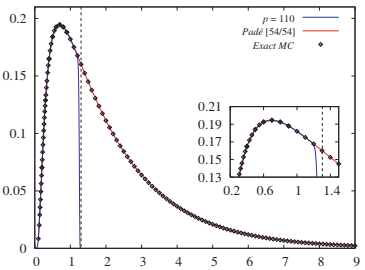

Fig 2: Amplitude $A(0,1,\beta)$ as a function of β for an anharmonic oscillator with quartic coupling k=0.4: N=1 p=110 approximation, Padé [54/54] approximant, and exact MC results. Vertical line is radius of convergence of small-time expansion.

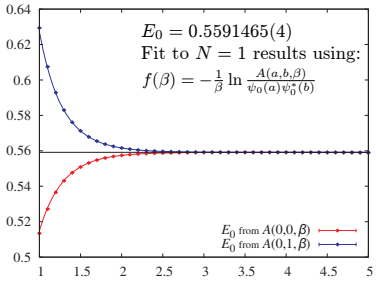

Fig. 3: Obtaining ground state energy from $f(\beta)$ for an anharmonic oscillator with the quartic coupling k=0.4.

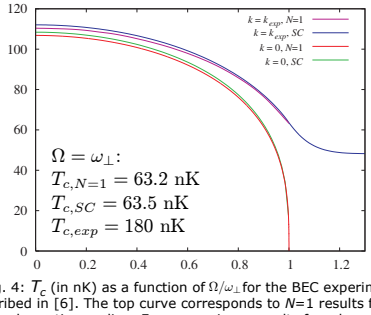

Fig. 4: T_c (in nK) as a function of $\Omega/\omega_\perp$ for the BEC experiment described in [6]. The top curve corresponds to N=1 results for the actual quartic coupling. For comparison, results for a harmonic trap are given in the bottom two curves. SC denotes semiclassical results of Ref. [7].

N=1 APPROXIMATION

- The accessibility of higher p effective actions allows a very accurate calculation of path integrals for small propagation times. It even allows the use of N=1 approximation (a single time-slice). In this approximation, the amplitudes are given as algebraic expressions, without any remaining integrals.
- While this approximation naturally works very well for $\varepsilon < 1$, it can be extended to larger propagation times using standard Padé approximants (Figs. 1, 2).
- The range of propagation times to which the N=1 approximation can be extended depends on the available number of terms in the effective action expansion.
- Using the new approach, we have calculated discretized effective actions for anharmonic oscillators up to order p=110. This makes it possible to substantially extend the propagation times, and to precisely calculate low-lying energy levels (Fig. 3).

APPLICATION TO BOSE-EINSTEIN CONDENSATION

- Rotation of Bose-Einstein condensate (BEC) adds angular momentum to the system. This can be compared to the motion of a charged particle in a magnetic field.
- In a recent experiment [6], a BEC of 3x10^5 ^{87}RB atoms was trapped in a quartic potential. The condensate was set into fast rotation, so that the centrifugal force compensated the harmonic part of the potential in the perpendicular plane, the confinement being ensured by the quartic part of the potential: $V = \frac{M}{2}(\omega_\perp^2 - \Omega^2)r_\perp^2 + \frac{M}{2}\omega_z^2 z^2 + \frac{k}{4}r_\perp^4$, where $\omega_\perp = 2\pi \times 64.8$ Hz, $\omega_z = 2\pi \times 11.0$ Hz, $k_{exp} = 2.6 \times 10^{-11}$ Jm^{-4}.
- Following the analysis of this system as a rotating ideal Bose gas [7], we have applied the newly developed N=1 path integral approximation to the calculation of the critical temperature for this system (Fig. 4) using SPEEDUP MC code [8].
- The obtained results are in good agreement with semiclassical ones obtained in [7]. For $\Omega = \omega_\perp$ (the actual experimental setup), we find $T_{c,N=1}$=*63.2(1)* nK, compared to $T_{c,SC}$=63.5 nK found in [7]. More detailed analysis will be presented in [9].
- Taken together, these results strengthen the case that new and more precise experimental measurements of the critical temperature need to be conducted, to understand the discrepancy between theory and $T_{c,exp}$ =180 nK reported in [6] .

SUMMARY

- We have presented a new recursive approach to the calculation of discretized effective actions leading to substantial, systematical speedup of numerical procedures for the calculation of path integrals of a generic many-particle non-relativistic theory.
- The new method allowed us to obtain higher order corrections to the ideal effective action (p>100), and in conjunction with Padé approximation it made it possible to calculate path integrals with high precision even in N=1 (one time-slice) approximation, effectively without any integrals.
- The presented N=1 approximation was successfully applied to the calculation of the critical temperature of a rotating BEC of ^{87}RB atoms trapped in a quartic potential.

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