Systematic Speedup of Many-Body Path Integral Calculations

I. Vidanović, A. Balaž, A. Bogojević, A. Belić

Institute of Physics Belgrade

http://scl.phy.bg.ac.yu/

Motivation

Path Integral Monte Carlo is the key numerical method for studying properties of quantum and statistical systems. However, PIMC simulations are notoriously demanding of computing time. We present a computation scheme that systematically and substantially improves convergence of general multi-particle simulations through the introduction of improved effective discretized actions.

1 INTRODUCTION

Quantum mechanical amplitudes are the continuum limit of discretized expressions of the form

$$A_N(q_i, q_f; \beta) = \left(\tfrac{1}{2\pi\varepsilon}\right)^{N/2} \int dq_1 \cdots dq_{N-1} e^{-S_N},$$

where S_N is the naively discretized action given in terms of $\bar{q}_n = \frac{1}{2}(q_n + q_{n+1})$, discretized velocities $\delta_n = q_{n+1} - q_n$ and time step $\varepsilon = \beta/N$.

Though well suited for numerical calculations, such expressions converge slowly to the continuum limit (typically as $1/N$).

We present and work with a scheme for improving the discretized action in a way that systematically speeds up convergence to $1/N^p$ for general p.

2 EFFECTIVE ACTIONS

- The underlying idea behind the construction of better discretizations (better effective actions) is to find a procedure for adding auxiliary counter terms that vanish in the continuum limit into the naively discretized action in such a way as to improve the convergence of general amplitudes.
- Previous methods for doing this were based on improving short-time propagator, generalizations of the Trotter-Suzuki formula, expansions in the number of derivatives, etc.
- Recently, the study of the relationship between discretizations of different coarseness has resulted in the construction of a hierarchy of effective discretized actions $S_N^{(p)}$ giving convergence $1/N^p$ [1-3]. Explicit analytical expressions for the effective actions were derived up to $p = 12$. This substantial speedup was up to now limited to physically relatively uninteresting one-particle systems.

3 NEW APPROACHES

- The existence and basic properties of the ideal discretized action S_N^* giving immediately the continuum result ($A_N^* = A$) were established in [4]. Applying the idea of relating different discretizations, the equation for S_N^* is easily obtained from:

$$A_{2N}^* = A_N^*$$

The above equation is solved approximately through asymptotic expansion in time step ε. The truncation of S_N^* to ε^p gives $S_N^{(p)}$.

- Another method to obtain ε-expanded S_N^* is to calculate the action in the path integral to the desired ε^p order using short-time approximation:

$$e^{-S^*} = A(\varepsilon)$$

Advantages:

- much simpler derivation
- easily generalizable to many-particle multi-dimensional systems
- different choices of referent trajectories recover other approximation techniques.

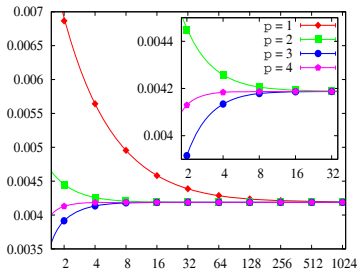
4 RESULTS

- We have introduced a new systematic approach for the derivation of effective discretized actions.
- The key new step is the generalization of the formalism to generic many-particle quantum mechanical systems in arbitrary dimensions.
- Explicit analytical expressions for the effective actions have been derived for $p \le 12$, i.e. converging as $1/N^{12}$.
- We have developed and tested a PIMC code that implements the newly derived effective actions.
- Using the new code we performed a series of extensive simulations calculating amplitudes, partition functions and energy spectra for various models. The obtained results verify the analytically derived increase in convergence, as can be seen in the presented figures.

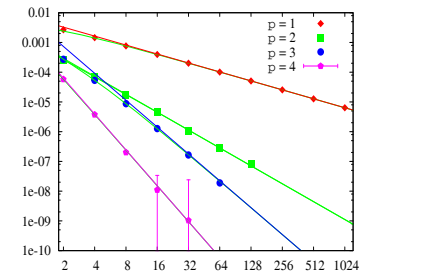
As an illustration, the $p = 4$ effective action is:

$$\begin{aligned} S_N^{(p=4)} = & \sum_n \left\{ \varepsilon \left(\frac{\delta_i \delta_i}{2\varepsilon^2} + V \right) \right. \\ & + \frac{\varepsilon^2}{12} \partial_{k,k}^2 V + \frac{\varepsilon \delta_i \delta_j}{24} \partial_{i,j}^2 V \\ & - \frac{\varepsilon^3}{24} \partial_i V \partial_i V + \frac{\varepsilon^3}{240} \partial_{i,i,j,j}^4 V + \frac{\varepsilon^2 \delta_i \delta_j}{480} \partial_{i,j,k,k}^4 V + \frac{\varepsilon \delta_i \delta_j \delta_k \delta_l}{1920} \partial_{i,j,k,l}^4 V \\ & + \frac{\varepsilon^4}{6720} \partial_{i,i,j,j,k,k}^6 V - \frac{\varepsilon^4}{120} \partial_i V \partial_{i,k,k}^3 V - \frac{\varepsilon^4}{360} \partial_{i,j}^2 V \partial_{i,j}^2 V \\ & - \frac{\varepsilon^3 \delta_i \delta_j}{480} \partial_k V \partial_{k,i,j}^3 V + \frac{\varepsilon^3 \delta_i \delta_j}{13340} \partial_{i,j,k,k,l,l}^6 V - \frac{\varepsilon^3 \delta_i \delta_j}{1440} \partial_{i,k}^2 V \partial_{i,j}^2 V \\ & \left. + \frac{\varepsilon^2 \delta_i \delta_j \delta_k \delta_l}{53760} \partial_{i,j,k,l,m,m}^6 V + \frac{\varepsilon \delta_i \delta_j \delta_k \delta_l \delta_m \delta_n}{322560} \partial_{i,j,k,l,m,n}^6 V \right\} \end{aligned}$$

5 RESULTS OF MONTE CARLO CALCULATIONS



Convergence of a typical discretized amplitude to the continuum as a function of level p for two-particle 2D system with quartic coupling.



Deviations of discretized amplitudes from the continuum limit on log-log scale. Solid lines represent the expected leading $1/N^p$ behavior.

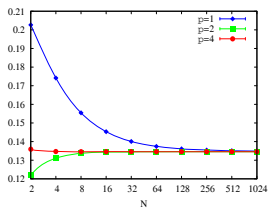
6 EFFICIENT CALCULATION OF ENERGY SPECTRA

Improved convergence of discretized amplitudes directly leads to the improved convergence of discretized partition functions.

The partition function is the central object for obtaining information about energy spectra.

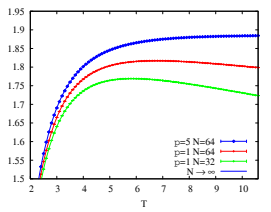
Higher level effective actions make it possible to determine energy levels using much coarser discretizations.

$$Z_N(\beta) = \int_{-\infty}^{\infty} dq A_N(q, q; \beta)$$

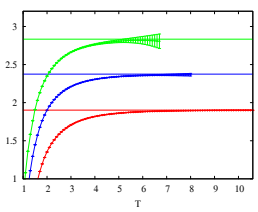


Convergence of a typical discretized partition function to the continuum with level p.

$$Z(\beta) = \sum_{n=0}^{\infty} d_n e^{-\beta E_n}$$



Free energy versus propagation time for different levels p and different discretizations.



Low lying energy levels determined using $p = 5$ and $N = 64$.

7 SUMMARY

- We have presented an algorithm that leads to substantial, systematical speedup of numerical procedures for the calculation of path integrals of a generic many-particle non-relativistic theory.
- Results hold for all path integrals - for transition amplitudes, partition functions, expectation values, as well as for calculations of energy levels.
- The developed calculation scheme has been completed and is ready for application to relevant problems condensed matter physics.
- The analytical work in progress will focus on generalization of the outlined scheme to more complex quantum systems: bosonic and fermionic quantum field theory, gauge theories, topologically non-trivial spaces, gravitation.

ACKNOWLEDGEMENTS

This work was supported in part by the Ministry of Science of the Republic of Serbia, under project no OI141035. I. Vidanović has received support under FP6 project CX-CMCS. The presented numerical results were obtained on the AEGIS e-Infrastructure whose operation is supported in part by FP6, projects, EGEE-II and SEE-GRID-2.

REFERENCES

[1] A. Bogojević, A. Balaž, A. Belić, *Phys. Lett. A* **344,** 84 (2005)

[2] A. Bogojević, A. Balaž, A. Belić, *Phys. Rev. Lett.* **94,** 180403 (2005)

[3] A. Bogojević, A. Balaž, A. Belić, *Phys. Rev. B* **72,** 064302 (2005)

[4] A. Bogojević, A. Balaž, A. Belić, *Phys. Rev. E* **72,** 036128 (2005)

[5] D. Stojiljković, A. Bogojević, A. Balaž, *Phys. Lett. A* **360**, 205 (2006)

[6] J. Grujić, A. Bogojević, A. Balaž, *Phys. Lett. A* **360**, 217 (2006)

[7] http://scl.phy.bg.ac.yu/speedup/