Path Integral Worm Algorithms

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Introduction to Computational Techniques to solving Path Integrals

Introduced in 1933 by Dirac, who speculated on the role that the action plays in quantum mechanics and properly formulated by Feynman in 1948, Path Integrals are now a third formulation of quantum mechanics. In essence they describe how all paths a particle can take contribute to the propagator describing the journey from a point to another. From field theory to statistical physics, they have turned out to be a useful technique to describe systems by providing a surprisingly intuitive way of viewing quantum mechanics. In this poster we will explore how we can leverage the power of Monte Carlo Worm algorithms to derive the thermodynamics of a Bose System in the Canonical Ensemble.

1. Path Integrals

Quantum path integrals, provide a unique and powerful method for analysing quantum systems by considering all possible paths that a particle can take in a given process.[1]

- In Classical Physics, the Principle of Least Action states that the true path of a particle is the one that minimizes the Action. In Quantum Mechanics, the Path Integral Formulation states that all possible paths contribute to a particle's behaviour and that each path has a complex probability amplitude assigned. When considering a large number of paths (classical limit), we retrieve the Principle of Least Action.
- We define the Propagator as the probability amplitude for a particle to travel from one place to another in a given period of time and that can be written as the Configuration Space Path Integral:

$$K(q_i, 0; q_f, T) = \int_{q(0)=q_i}^{q(T)=q_f} Dq(t) e^{iS[q(t)]} \quad \text{where} \quad S(q) = \int_{t_i}^{t_f} \mathcal{L} dt \quad \text{is the Action.} \tag{1}$$

2. Worm Algorithms

A few definitions:

- Monte Carlo Simulations: Estimate the possible outcomes of an uncertain event based on a set of fixed input values.
- Markov Chain: Stochastic model where the probability of each event depends only on the previous event.

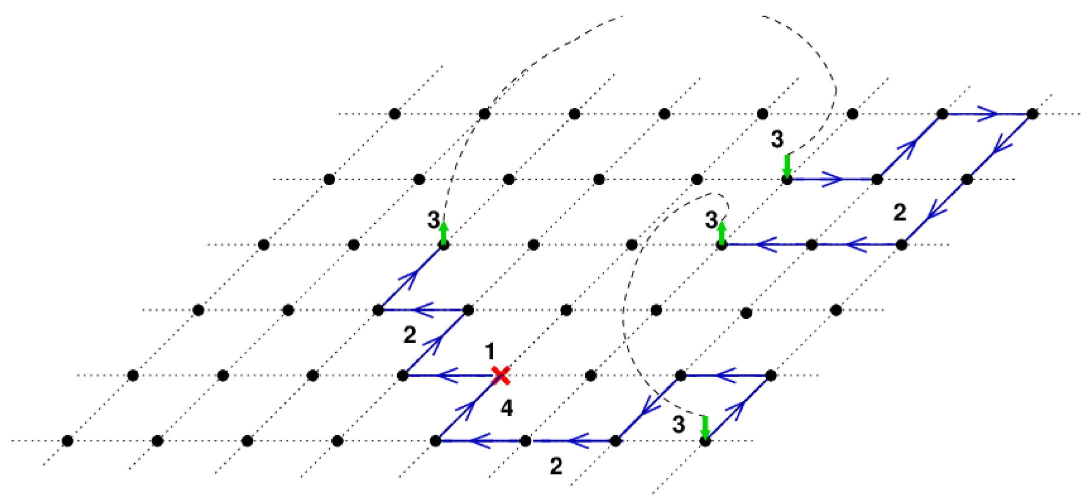

Fig. 1: Illustration of a Worm Algorithm exploring the space of possible world lines/configurations.

Worm Algorithms[2] explore the space of possible world lines/paths a system can move one by creating/annihilating pairs of "Worms", representing fictitious endpoints of open word lines. They stochastically move through the lattice, exploring configurations of these lines and annihilate each other when two endpoints meet.

- The algorithms generate samples of valid world lines that follow the probability distribution of a quantum system dictated by the path integral.
- Worm Algorithms provide a way to numerically evaluate the expectation values of observables by sampling the statistical ensemble of a quantum system.
- They do not compute the integrals directly but rather describe the space of path configuration associated with a path integral.

3. Bose Systems in the Canonical Ensemble

- Bose systems describe collections of non-interaction, indistinguishable particles occupying discrete energy states at thermodynamic equilibrium.
- In Statistical Physics, the Canonical Ensemble represents the possible states of a system in thermal equilibrium. It can exchange energy with its surroundings.

Here will aim at calculating the partition function Z_N of N indistinguishable particles, with Hamiltonian H and inverse temperature $\beta = \frac{1}{k_B T}$. The partition function is defined by:

$$Z_N = tr(e^{-\beta \hat{H}}) = \frac{1}{\hbar N!} \int dq dp \langle q, p| e^{-\beta \hat{H}} \; q, p \rangle \tag{2}$$

4. Application

We can use the Worm Algorithm as a Monte Carlo method that sample permutations (exchange of any two identical particles) in the Bose systems where the simulation cell has a lattice-like structure with periodic boundary conditions. The algorithm generates new configurations that sample permutations in Bose systems. Here is the general algorithm detailed[3]:

1. Initialise the system with a given number of particles and periodic boundaries for the lattice.
2. Choose an initial permutation of the particles.
3. Perform a series of elementary moves on the permutation.
4. Calculate the Energy for each new configuration generated by the moves.
5. Accept or reject each move based on its probability. If it is accepted, the configuration is considered achievable for the given system.
6. Repeat the last 3 steps until we have mapped enough possible configurations.
7. We can now use those configurations to determine statistical averages and thus thermodynamic properties such as the partition function, free energy, and specific heat.

5. Results

Spada, Giorgini and Pilati [3] benchmark the performance of the Worm Algorithm against the know exact results of the non-interaction Bose gas for one, two and many particles at various temperatures.

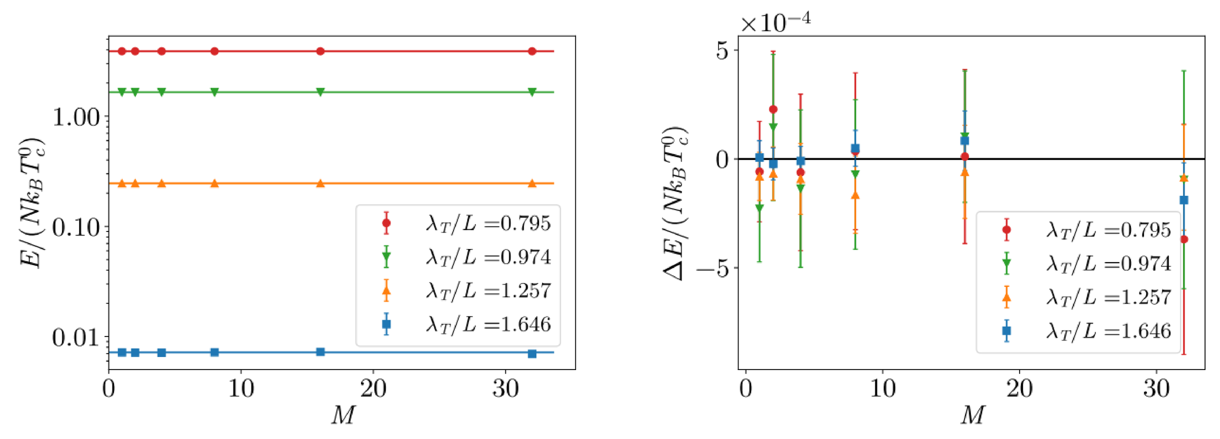

Fig. 2: Results for a single particle. Left: Internal Energy for a different number of measurements compared to the exact results (horizontal lines). Right: Differences with the exact values.

We observe that the results fit with great accuracy the actual results. For two and three particles, there are no exact solutions available but we can compare the Worm Algorithm with other numerical methods. The conclusion is that the Worm Algorithm is a powerful method compared to the Path Integral Monte Carlo methods but its performance greatly depends on the specific problem being studied.

6. Other computational techniques

There are other powerful quantum algorithms that are related to Path Integrals, their usage or their calculation. The Metropolis Algorithm that is also used to sample world line configurations, enabling the estimation of expectation values. The Path Integral Monte Carlo evaluates finite-temperature path integrals for quantum systems, which is useful when studying fluids and gases.

References

[1] Richard MacKenzie. *Path Integral Methods and Applications*. 2000. arXiv: `quant-ph/0004090 [quant-ph]`.

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[3] Gabriele Spada, Stefano Giorgini, and Sebastiano Pilati. "Path-Integral Monte Carlo Worm Algorithm for Bose Systems with Periodic Boundary Conditions". In: *Condensed Matter* 7.2 (Mar. 2022), p. 30. DOI: `10.3390/condmat7020030`. URL: `https://doi.org/10.3390%2Fcondmat7020030`.

[4] Marise J. E. Westbroek et al. "User's guide to Monte Carlo methods for evaluating path integrals". In: *American Journal of Physics* 86.4 (Apr. 2018), pp. 293–304. DOI: `10.1119/1.5024926`. URL: `https://doi.org/10.1119%2F1.5024926`.