The density of states from first principles

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Motivations

- Monte-Carlo simulations are the very effective for observables that can be written as expectation values over a probability measure.

$$\hat{O} = \langle O \rangle \tag{1}$$

- They are not as efficient when they deal with free energies or partition functions. [1]

- They are not suitable for system with complex action.

[1] P. de Forcrand, M. D'Elia, and M. Pepe, Phys.Rev.Lett. 86 , 1438

The density of states

- Let us consider an euclidean quantum fied theory

$$Z = \int [D\phi] e^{-\beta S[\phi]} \tag{2}$$

- The density of states is defined as

$$\rho(E) = \int [D\phi] \delta(S[\phi] - E) \tag{3}$$

- Which leads to

$$\langle O \rangle = \frac{\int \rho(E) O(E) e^{-\beta E}}{\int \rho(E) e^{-\beta E}} \tag{4}$$

Algorithm for the density of states

- If the density of states is known then free energies and expectation values are accessible via a simple integration.
- The Wang-Landau algorithm is a numerical technique to extract the density of states in statistical mechanics.
- A direct generalization to continuum system does not seem very efficient. [2]

[2] J. Xu and H.-R. Ma, Phys.Rev. E75, S. Sinha and S. Kumar Roy, Phys.Lett. A373

A novel algorithm for continuous model

- If we rescrict the energy interval to a small interval 2Δ, we have

$$\langle\langle f(E)\rangle\rangle_a = \frac{1}{Z}\int_{E_0-\Delta}^{E_0+\Delta} f(E)\rho(E)e^{-aE}dE \tag{5}$$

- If the interval is small enough we can approximate $\log(\rho)$ with a linear function

$$\rho(E)\exp(-aE) = constant + \mathcal{O}(\Delta) \tag{6}$$

- Which derived gives

$$a(E_0) \sim \left.\frac{d\log\rho}{dE}\right|_{E=E_0} \tag{7}$$

- Our goal will be to compute the coefficients a.

A novel algorithm for continuous model

- We can choose $f(E) = \Delta E = E - E_0$ we will have

$$\langle\langle \Delta E \rangle\rangle_a = \frac{1}{Z} \int_{E_0-\Delta}^{E_0+\Delta} (E - E_0)\rho(E) e^{-aE} dE = \Delta E(a) \qquad (8)$$

- If the linear approximation we should be able to choose a such that

$$\rho(E) \exp(-aE) = constant + \mathcal{O}(\Delta) \qquad (9)$$

- Which gives

$$\langle\langle \Delta E \rangle\rangle_a = 0 \qquad (10)$$

A modified Wang-Landau algorithm

- The double brackets expectation values can be obtained efficiently by a standard Montecarlo that samples the configuration with weight

$$W(E) \propto e^{-aE}(\theta(E - E_0 + \Delta) - \theta(E - E_0 - \Delta)) \qquad (11)$$

- We need to find the coefficient a^* such that this Montecarlo procedure gives

$$\langle\langle \Delta E \rangle\rangle_{a^*} = 0 \qquad (12)$$

- This is a root finding problem.

The Newton-Raphson procedure

- A simple procedure to find the root of a function is the iterative Newton-Raphson method

$$a_{n+1} = a_n - \frac{\langle\langle \Delta E \rangle\rangle_{a_n}}{\langle\langle \Delta E \rangle\rangle'_{a_n}} \sim a_n - \frac{3\langle\langle \Delta E \rangle\rangle_{a_n}}{\Delta^2} \tag{13}$$

- While this algorithm seems to work fine and to give correct results, we are not considering that we cannot compute $\langle\langle \Delta E \rangle\rangle$ exactly, but we can only estimate it via noisy Montecarlo simulations.
- We are not able to provide a mathematical proof of convergence.

Robbins-Monro method

- The Robbins and Monro algorithm [3] is specifically designed to find the root of a function $f(x)$ that cannot be computed exactly but we can obtain measurments $m(x)$ such that $\langle m(x)\rangle = f(x)$
- The iterative algorithm has the form

$$a_{n+1} = a_n - c_n \langle\langle \Delta E \rangle\rangle_{a_n} \tag{14}$$

where

$$\sum_{n=0}^{\infty} c_n = \infty; \quad \sum_{n=0}^{\infty} c_n^2 < \infty; \tag{15}$$

[3] Robbins, H.; Monro, S. (1951). The Annals of Mathematical Statistics 22

Robbins-Monro method

- Robbins-Monro proved that

$$a_n \underset{a.s.}{\rightarrow} a^* \tag{16}$$

- Moreover a_n is (asymptotically) distributed normally around a^*.
- From the knowledge of the coefficients $a^*(E_0^i)$ it is simple to reconstruct the density of states, the simplest possible formula is

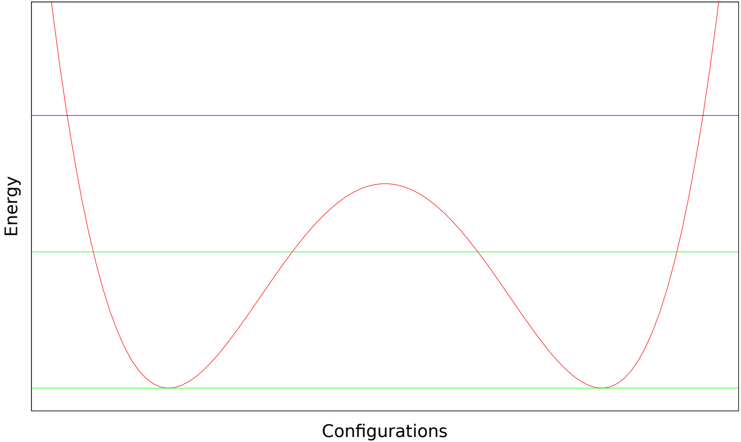
$$\rho(E) = \prod_{i=1}^{k} e^{a^*(E_0^i)\Delta} exp(a^*(E_0)(E - E_0^k)) \tag{17}$$

with

$$E_0^k \leq E < E_0^{k+1} \tag{18}$$

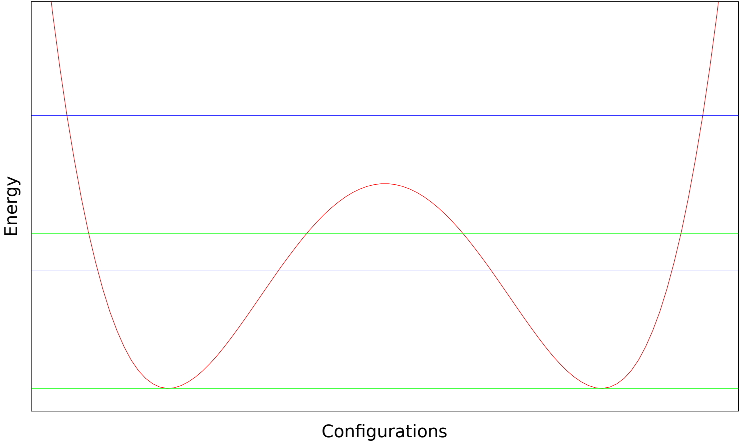
Rugged energy landscape

- What if the energy landscape is rugged?



Parallel tempering

- Overlapping energy intervals



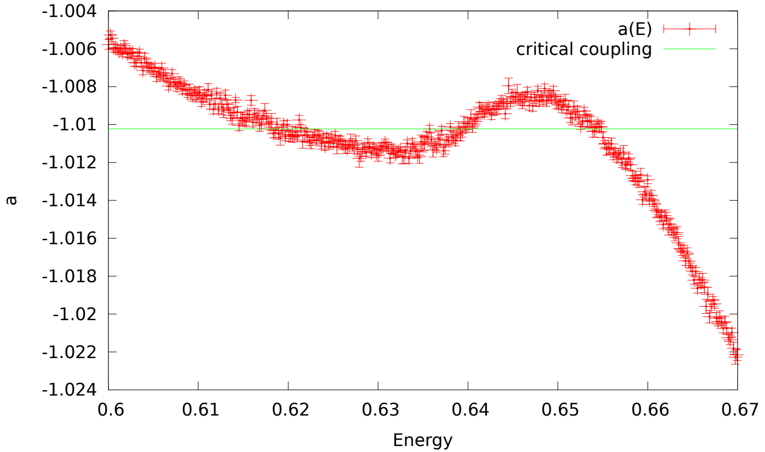
Parallel tempering

- When two systems in different energy intervals are in the overlapping region swap with probability

$$P_{sw} = \min(1, \exp(\Delta a \Delta E)) \tag{19}$$

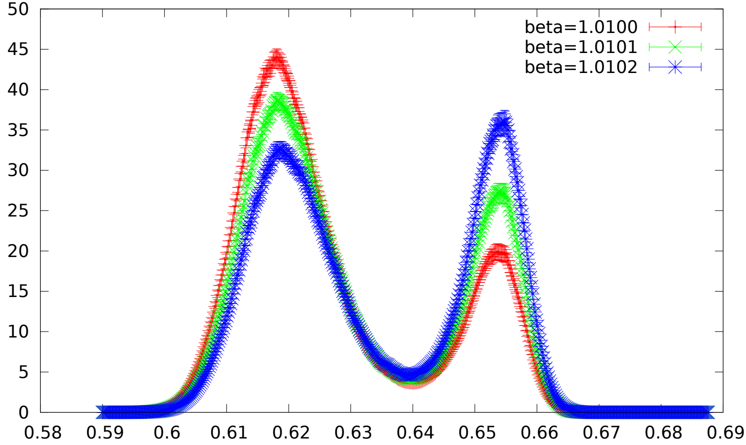
Compact $U(1)$

- We tested our approach for the compact $U(1)$ lattice gauge theory.



Compact $U(1)$

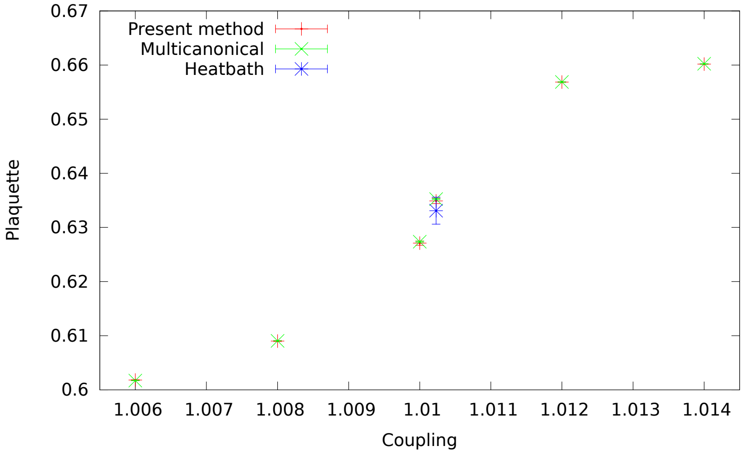
- The system is known to possesses a first order phase transition [4].



[4] G. Arnold, B. Bunk, T. Lippert, and K. Schilling, Nucl.Phys.Proc.Suppl. 119

Compact $U(1)$

- Plaquette near the critical region



Conclusions

- We proposed a novel approach to compute the Density of states in theories with coninuum deegres of freedom.
- We believe that it could be very useful to study observables related to free energies such as interface tensions or monopole masses.
- Moreover as the density of states is real can be used also for theories with a sign problem.