The density of states from first principles

Roberto Pellegrini

1Department of Physics, Swansea University, Singleton Park, Swansea, SA2 8PP UK

In collaboration with K. Langfeld, B. Lucini, A. Rago
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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.

\[ \hat{O} = \langle O \rangle \]  (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.

¹P. 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. \(^2\)

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\(^2\) 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 restrict the energy interval to a small interval $2\Delta$, we have

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

(5)

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

$$\rho(E) \exp(-aE) = constant + O(\Delta)$$

(6)

- Which derived gives

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

(7)

- Our goal will be to compute the coefficients $a$. 

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A novel algorithm for continuous model

- We can choose \( f(E) = \Delta E = E - E_0 \) we will have
  \[
  \langle \langle \Delta E \rangle \rangle_a = \frac{1}{Z} \int_{E_0-\Delta}^{E_0+\Delta} (E - E_0) \rho(E) e^{-aE} dE = \Delta E(a) \tag{8}
  \]

- If the linear approximation we should be able to choose \( a \) such that
  \[
  \rho(E) \exp(-aE) = constant + O(\Delta) \tag{9}
  \]

- Which gives
  \[
  \langle \langle \Delta E \rangle \rangle_a = 0 \tag{10}
  \]
The double brackets expectation values can be obtained efficiently by a standard Montecarlo that samples the configuration with weight

$$W(E) \propto e^{-aE} \left( \theta(E - E_0 + \Delta) - \theta(E - E_0 - \Delta) \right)$$  \hspace{1cm} (11)

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

$$\langle \langle \Delta E \rangle \rangle_{a^*} = 0$$  \hspace{1cm} (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

\[ a_{n+1} = a_n - \frac{\langle \Delta E \rangle_{a_n}^a}{\langle \Delta E \rangle_{a_n}'} \sim a_n - \frac{3\langle \Delta E \rangle_{a_n}}{\Delta^2} \]  \hspace{1cm} (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.
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 measurements \(m(x)\) such that \(\langle m(x) \rangle = f(x)\).

The iterative algorithm has the form

\[
a_{n+1} = a_n - c_n \langle \langle \Delta E \rangle \rangle_{a_n}
\]

where

\[
\sum_{n=0}^{\infty} c_n = \infty; \quad \sum_{n=0}^{\infty} c_n^2 < \infty;
\]

\(^3\)Robbins, H.; Monro, S. (1951). The Annals of Mathematical Statistics 22.
Robbins-Monro method

- Robbins-Monro proved that

\[ a_n \to a^* \quad \text{a.s.} \tag{16} \]

- 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

![Energy vs Configurations Diagram](image-url)
Parallel tempering

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

\[ P_{sw} = \min(1, \exp(\Delta a \Delta E)) \] (19)
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 \(^4\).

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\(^4\)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 continuum degrees 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.