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# Efficient computations of continuous action densities of states for lattice models

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**Abstract.** The Logarithmic Linear Relaxation (LLR) algorithm is an efficient method for computing densities of states for systems with a continuous spectrum. A key feature of this method is exponential error reduction, which allows us to evaluate the density of states of a system over hundreds of thousands of orders of magnitude with a fixed level of relative accuracy. As a consequence of exponential error reduction, the LLR method provides a robust alternative to traditional Monte Carlo calculations in cases in which states suppressed by the Boltzmann weight play nevertheless a relevant role, e.g., as transition regions between dominant configuration sets. After reviewing the algorithm, we will show an application in U(1) Lattice Gauge Theory that has enabled us to obtain the most accurate estimate of the critical coupling with modest computational resources, defeating exponential tunneling times between metastable vacua. As a further showcase, we will then present an application of the LLR method to the decorrelation of the topological charge in SU(3) Lattice Gauge Theory near the continuum limit. Finally, we will review in general applications of the LLR algorithm to systems affected by a strong sign problem and discuss the case of the Bose gas at finite chemical potential.

## 1. Introduction

Markov Chain Monte Carlo (MCMC) are particularly well suited in calculations in which ensemble averages of extensive quantities that can be expressed explicitly as a function of the fields need to be computed. While cases in this category cover a good cross-section of relevant quantities in physics, they are by no means exhaustive. In fact, there are various scenarios, ranging from computations of partition functions to the sign problem, in which MCMC are inefficient. In this contribution, we will review the Logarithmic Linear Relaxation (LLR) algorithm, which enables us to overcome the limitations of MCMC methods in the presence of small overlaps between domains of relevant configurations. The superior performance of this

algorithm is provided by exponential error reduction[1], which is a central feature of the method.

This proceeding is organised as follows. We will present the LLR algorithm for real action systems and provide some example applications in Sect. 2. In Sect. 3, we will formulate the algorithm for complex action systems and discuss its application in a numerical study of the Bose gas at finite chemical potential, which is a popular benchmark model for assessing the efficiency of an algorithm at circumventing the sign problem. Sect. 4 will summarise our contribution and outline some further directions of investigation.

## 2. The LLR algorithm for real action systems

Let us start by considering an Euclidean quantum field theory[2] written in a general form, whose path integral is given by the expression

$$Z(\beta) = \int [D\phi] e^{-\beta S[\phi]} \ . \tag{1}$$

Here, $\phi$ is a field configuration over a lattice $\Lambda$, $\beta$ is the coupling and $S$ the action. The integral is performed over all possible values of the fields. The density of states associated to a value $E$ of the action $S$ of the model is defined as

$$\rho(E) = \int [D\phi] \delta(S[\phi] - E) \ . \tag{2}$$

Using this expression for $\rho$, we can reformulate the path integral as an integral over all possible energy values weighted by the density of states and the Boltzmann measure:

$$Z(\beta) = \int dE \rho(E) e^{-\beta E} = e^{-\beta F} \ . \tag{3}$$

If the density of states is known, free energies and expectation values are accessible via simple numerical integrations. For instance, for an observable that depends only on $E$,

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

Therefore, an algorithm that enables us to compute $\rho(E)$ will straightforwardly give us access, through a numerical integration, to the free energy $F$ and to values of thermodynamic ensemble averages of observables depending on $E$ as a function of $\beta$. For systems with discrete energy levels, an algorithm of this type, the celebrated Wang-Landau algorithm, was provided in [1]. The LLR method, which was inspired by the latter work, is an algorithm for the calculation of densities of states in systems with a continuous spectrum [2, 3]. This algorithm is implemented as follows. We start by dividing the (continuum) energy interval of the system in $N$ sub-intervals of amplitude $\delta_E$, with the interval $n$ centered at the value $E_n$. We then define a piecewise continuous local linear approximation of $\log \rho(E)$ as

$$\log \tilde{\rho}(E) = a_n (E - E_n) + c_n \qquad \text{for } E_n - \delta_E/2 \leq E \leq E_n + \delta_E/2 \ , \tag{5}$$

which is valid for sufficiently small width $\delta_E$ of the energy sub-intervals. We obtain $a_n$ as the root of the stochastic equation

$$\langle\langle \Delta E \rangle\rangle_{a_n} = \int_{E_n - \frac{\delta_E}{2}}^{E_n + \frac{\delta_E}{2}} (E - E_n) \rho(E) e^{-a_n E} dE = 0 \tag{6}$$

[1] We use the expression *exponential error reduction* to indicate that the relative error of a quantity is independent from the value of the latter.

[2] Although for the sake of definiteness in this work we use the language of Euclidean quantum field theories, a translation of the method to a statistical mechanics context is immediate.

using the Robbins-Monro iterative method [4]

$$\lim_{m\to\infty} a_n^{(m)} = a_n \ , \qquad a_n^{(m+1)} = a_n^{(m)} - \frac{\alpha}{m} \frac{\langle\langle \Delta E \rangle\rangle_{a_n^{(m)}}}{\langle\langle \Delta E^2 \rangle\rangle_{a_n^{(m)}}} \ , \qquad \alpha \text{ constant} \ . \tag{7}$$

In Eqs. (6) and (7) we have used the double-angle notation for the expectation of an observable $O(E)$, which is defined as

$$\langle\langle O(E) \rangle\rangle_{a_n} = \frac{1}{\mathcal{N}} \int_{E_n - \frac{\delta_E}{2}}^{E_n + \frac{\delta_E}{2}} O(E) \rho(E) e^{-a_n E} dE \ , \qquad \mathcal{N} = \int_{E_n - \frac{\delta_E}{2}}^{E_n + \frac{\delta_E}{2}} \rho(E) e^{-a_n E} dE \ . \tag{8}$$

These energy-restricted integrals can be easily reformulated as integrals over the all spectrum with sharp cut-offs provided by appropriate Heaviside functions. These sharp cut-offs can be replaced with a smooth Gaussian cut-off [5]. The double-angle expectations are computed with a MCMC restricted to the relevant energy interval. Note that if we repeat the Robbins-Monro algorithm starting from different random numbers, asymptotically, at fixed number of iterations $m$, the $a_n^{(m)}$ are gaussianly distributed around the root $a_n = a_n^{(\infty)}$ with a variance that goes to zero as $m$ increases. This property provides an immediate strategy for converting potential systematic errors into statistical errors in the root finding procedure.

After computing the $a_n$ for all $n$, setting $c_1 = 0$, the piecewise continuity of $\log \tilde{\rho}(E)$ gives

$$c_n = \frac{\delta}{2} a_1 + \delta \sum_{k=2}^{n-1} a_k + \frac{\delta}{2} a_n \ , \qquad n \geq 2 \ . \tag{9}$$

The numerically determined $\tilde{\rho}(E)$ can be used in path integral calculations *in lieu* of $\rho(E)$. This procedure result in a systematic approximation error in $\delta_E$ that is however controlled, since it scales quadratically with the width of the sub-intervals. Remarkably, our procedure for determining $\tilde{\rho}$ provides exponential error suppression [3]. It is worth noting that the restricted sampling discussed above is non-ergodic. Ergodicity can be recovered using the replica exchange method, as discussed in [6].

Exponential error suppression has been proved to be spectacularly implemented in the method in [2], where, using the piecewise continuous density of states that has been reconstructed over 250000 orders of magnitude, it has been shown that the LLR-determined SU(3) lattice gauge theory plaquette agrees with MCMC calculations over a wide range of $\beta$ values that interpolate between the strong coupling and the weak coupling regime of the theory.

Due to the presence of a first-order deconfinement phase transition, a notoriously hard to simulate system is compact U(1) lattice gauge theory. The best available MCMC calculations used a large amount of computer time on then state-of-the-art supercomputers, reaching a maximum lattice size of $18^4$ when periodic boundary conditions were imposed [7]. Using the LLR algorithm, we were able to perform accurate and robust calculations with moderate computational resources on a $20^4$ lattice [3]. A reconstruction of the probability distribution of the energy at the pseudocritical value of $\beta$ obtained on our largest system with the LLR algorithm is shown in Fig. 1.

More recently, we have shown in [8] that the LLR algorithm mitigates significantly the problem of the topological freezing [9] by performing a calculation of the correlation time of the topological charge in SU(3) pure gauge theory near the continuum limit. Fig. 2 shows that, compared to MCMC methods, the LLR algorithm reduces this correlation time by about one order of magnitude.

Other successful applications of the LLR method include the calculation of the order-disorder interface tension in the Potts model [6] and the calculation of the renormalisation constant for the energy-momentum tensor in SU(2) lattice gauge theory using the method of shifted boundary conditions, which in turn requires computations of free energies from partition functions [5].

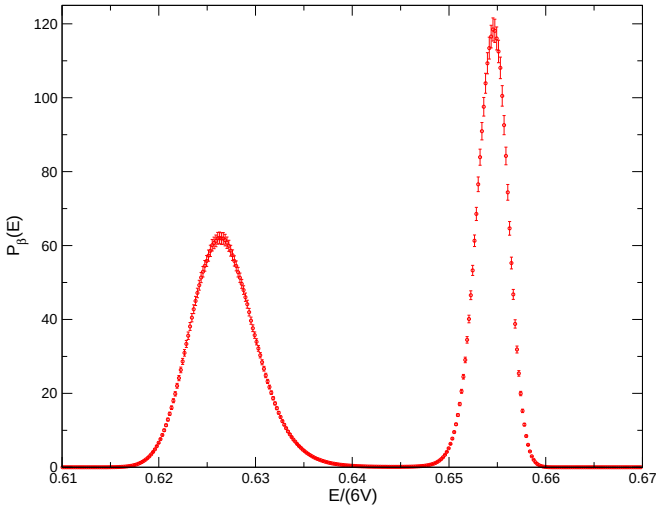


**Figure 1.** Probability distribution of the energy $E$ for compact U(1) lattice gauge theory at $\beta = 1.011006$ (central estimate for the critical value using the latent heat peak) on a $20^4$ lattice.

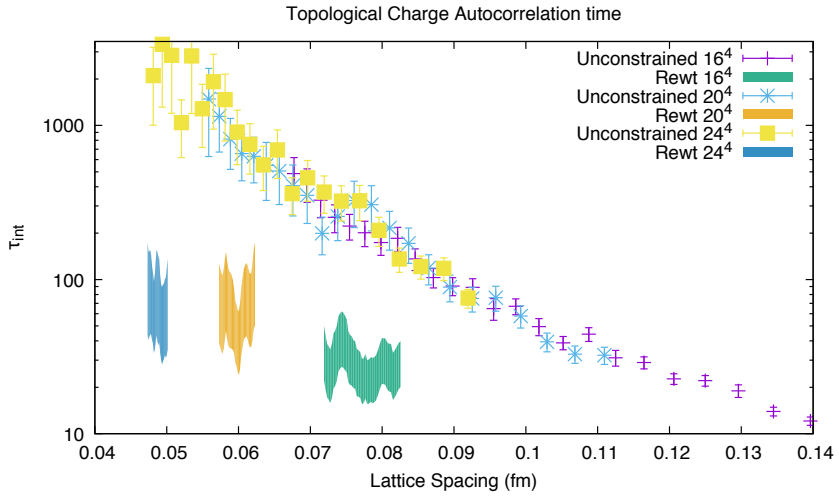


**Figure 2.** Correlation time of the topological charge for SU(3) gauge theory at the lattice volumes shown as a function of the lattice spacing. The "unconstrained" points are obtained with a standard heat bath method, while the "rewt" points come from LLR simulations.

## 3. The LLR algorithm for complex action systems

We now consider an Euclidean quantum field theory with a complex action, whose path integral we write as

$$Z(\mu) = \int [D\phi] e^{-\beta S[\phi] + i\mu Q[\phi]} \ . \tag{10}$$

The generalised density of states is defined as

$$\rho(q) = \int [D\phi] e^{-\beta S[\phi]} \delta(Q[\phi] - q) \ . \tag{11}$$

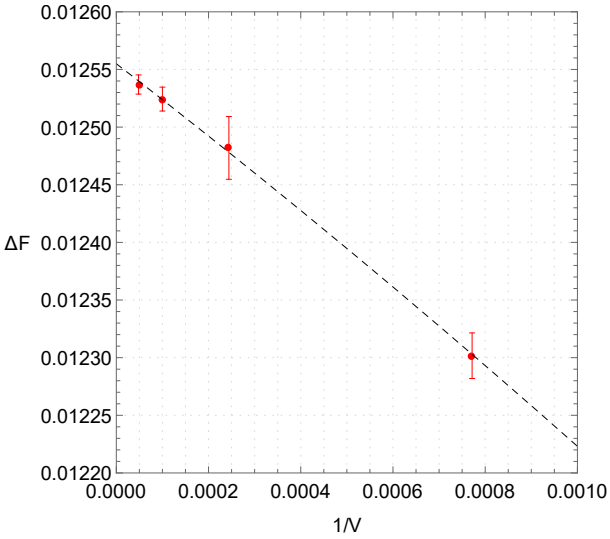


**Figure 3.** Computation of the overlap free energy for the Bose gas at finite chemical potential for various volumes. A linear extrapolation in $1/V$ to the thermodynamic limit is also shown.

In terms of $\rho(q)$, we rewrite $Z$ as

$$Z(\mu) = \int dq \rho(q) e^{i\mu q} \ . \tag{12}$$

In general, the above integral is strongly oscillating, These oscillations generate the large cancellations typical of a sign problem scenario. Because of the latter, when performing a calculation $\rho(q)$ in general needs to be known with an extraordinary degree of accuracy.

The severity of the sign problem is indicated by the *vev* of the phase factor in the phase quenched ensemble:

$$\langle e^{i\mu q} \rangle = \frac{Z(\mu)}{Z(0)} = e^{-V\Delta F} \to 0 \qquad \text{exponentially in } V \ . \tag{13}$$

Eq. (13) shows that the sign problem can be reformulated as an *overlap problem*, as the ensemble average of the phase factor depends on the overlap of relevant configurations for two different partition functions, which is exponentially suppressed with the volume. Since the LLR method has proved to be very efficient at computing regions with suppressed densities, it is natural to explore how it performs in this case[3]. We note though that, while the computation of the density is in the scope of the LLR algorithm, integration is a separate problem. In particular, in the complex case, it has been shown in [11] that a piecewise approximation of $\rho$ does not provide sufficient precision for computing relevant observables. In the same work, using a $Z(3)$ spin model as a prototype system, the authors showed that a polynomial interpolation of $\rho$ can be performed that is stable against the order of the interpolation and at the same time provides the required accuracy[4].

More recently, the method has been applied to the four-dimensional Bose gas system at finite chemical potential [13]. Fig. 3 shows the computation of the overlap free energy $\Delta F$ as a function

[3] A method for calculations of densities of states for systems with complex actions that is similar in spirit to the LLR algorithm is the FFA method, first proposed in [10].

[4] See [12] for a related proposal for the interpolation of the density based on a cumulant expansion.

of the volume $V$ for the latter system at chemical potential $\mu = 0.8$. Volumes up to the size $V = 16^4$ have been used. A linear extrapolation in $1/V$ (also reported in the figure) gives

$$\Delta F = (0.012557 \pm 0.000004) - \frac{(0.329 \pm 0.008)}{V} \ , \tag{14}$$

whose infinite volume limit is reassuringly close to the mean-field result $\Delta F_{MF} \simeq 0.012522$ computed in [14]. At the same time, the LLR result is sufficiently accurate to expose the expected deviations from the mean-field value.

## 4. Conclusions

The LLR algorithm enables accurate computations of density of states that can be used for precise calculations in scenarios in which MCMC are known to be inefficient. In this contribution, we have reviewed in particular some applications to first-order phase transitions, to the decorrelation of the topological charge and to the sign problem. A natural future direction is an extension to the algorithm to systems with fermions [15].

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