# The density of states in gauge theories

Langfeld, K; Lucini, B; Rago, A

**Published in:**
Phys.Rev.Lett.

**Publication date:**
2012

# The density of states in gauge theories

Kurt Langfeld[a], Biagio Lucini[b], and Antonio Rago[a]

[a] School of Computing & Mathematics, Plymouth, PL4 8AA, UK and
[b] College of Science, Swansea University, Swansea, SA2 8PP, UK

(Dated: March 19, 2012)

The density of states is calculated for a SU(2) and a compact U(1) lattice gauge theory using a modified version of the Wang-Landau algorithm. We find that the density of states of the SU(2) gauge theory can be reliably calculated over a range of 120,000 orders of magnitude for lattice sizes as big as $20^4$. We demonstrate the potential of the algorithm by reproducing the SU(2) average action, its specific heat and the critical couplings of the weak first order transition in U(1).

PACS numbers: 11.15.Ha, 12.38.Aw, 12.38.Gc



Monte-Carlo simulations [1] of the theory discretised on a Euclidean space-time lattice [2] currently provide the most successful approach to calculations from first principles in asymptotically free gauge theories in the energy domain in which the coupling is of order one. Although this strategy is successful for computations of observables that can be expressed as a vacuum expectation value (*vev*) on a theory with a semi-positive definite path integral measure, when the observable is not a *vev* (e.g., the free energy, which is related to the logarithm of a partition function) or the path-integral measure is not semi-positive (like in QCD at finite density), Monte-Carlo algorithms are either unsuitable or very inefficient.

An alternative numerical approach to Lattice Gauge Theories potentially free from those limitations is based on the density of states. Let us consider a quantum field theory with action $\beta S[\phi]$, with $\beta$ the inverse coupling. For this theory, the path integral in Euclidean space-time is given by

$$Z = \int \mathcal{D}\phi(x)\, \mathrm{e}^{\beta S[\phi]} \;, \tag{1}$$

where $(\mathcal{D}\phi(x))$ means that the integral has to be performed over all allowed configurations of the field $\phi$. Defining the density of states $\rho(E)$ as

$$\rho(E) = \int \mathcal{D}\phi(x)\; \delta(S[\phi] - E) \;, \tag{2}$$

the path integral can be rewritten as

$$Z = \int \rho(E) \mathrm{e}^{\beta E}\, \mathrm{d}E \,, \tag{3}$$

and the *vev* of an observable $O(E)$ becomes

$$\langle O \rangle = \frac{1}{Z} \int \rho(E)\, O(E)\, \mathrm{e}^{\beta E}\, \mathrm{d}E \;. \tag{4}$$

If the density of states is known, the path integral and $\langle O \rangle$ can be obtained by computing numerically or analytically respectively the integral (3) and (4).

An efficient algorithm for computing $\rho(E)$ in systems with discrete energy levels has been proposed by Wang and Landau in [3]. To date, the method has found various applications in Statistical Mechanics, some of which have produced remarkable results that can not be obtained with a direct Monte-Carlo approach (see e.g. [4] for a recent example). Despite its popularity in Statistical Mechanics, the Wang-Landau algorithm has found only limited applications in Lattice Gauge Theory [5, 6]. In fact, the sampling of a continuous density of states with a straightforward generalisation of the method given in [3] turns out to be problematic [7, 8]. In this work, we propose a new method for determining a continuous density of states and we apply it to calculate the density of states in SU(2) and U(1) on the lattice.

Throughout this paper we adopt the lattice regularisation, which leaves us with a $N^4$ cubic lattice as the discretisation of the Euclidean space-time. The dynamical degrees of freedom of the SU($N_c$) gauge theory are represented by the matrices $U_\mu(x) \in \mathrm{SU}(N_c)$, which are associated with the links of the lattice. We are using the so-called Wilson action, i.e.,

$$S[U] = \sum_{\mu>\nu,x} \frac{1}{N_c} \mathrm{Re}\,\mathrm{tr}\Big[ U_\mu(x)\, U_\nu(x+\mu)\, U_\mu^\dagger(x+\nu)\, U_\nu^\dagger(x) \Big], \tag{5}$$

stressing however that our approach is not limited to this particular action, but can handle e.g. improved actions equally well.

In order to present our novel type of numerical algorithm to calculate the density of states, we will assume that $\ln \rho(E)$ is well approximated by piecewise linear functions. It will indeed turn out below that $\ln \rho(E)$ is a remarkable smooth function of $E$.

Let us consider the energy interval $[E_0, E_0 + \delta E]$ for which we approximately write

$$\rho(E) \;=\; \rho(E_0)\, \exp\Big\{ a(E_0)\, (E - E_0) \Big\} \tag{6}$$

for $E_0 \le E < E_0 + \delta E$. Our goal will be to calculate the coefficients $a(E_0)$, which can be considered as derivatives of the density of states:

$$a(E_0) \;=\; \frac{\mathrm{d}\, \ln \rho(E)}{\mathrm{d}E}\Big|_{E=E_0} \;. \tag{7}$$

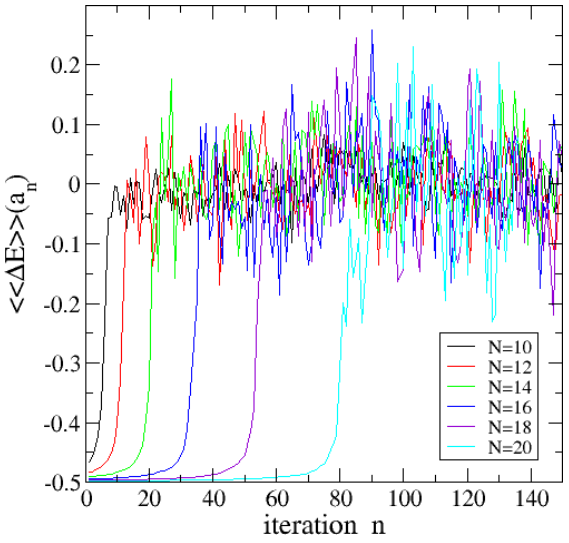


FIG. 1. The thermalisation history for a SU(2) gauge theory for lattice sizes $10^4 \ldots 20^4$.

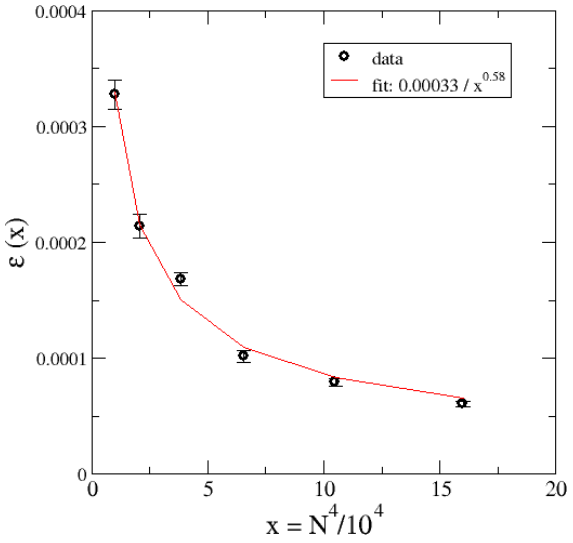


FIG. 2. The statistical error for the estimate of $a(E_0)$ for lattice sizes $10^4 \ldots 20^4$.

The strategy to obtain these coefficients is based upon the truncated and re-weighted expectation values defined by

$$\langle\!\langle f(E)\rangle\!\rangle(a) = \frac{1}{\mathcal{N}} \int \mathrm{d}E\; f(E)\; \rho(E)\, \theta_{[E_0,\delta E]}\;\; \mathrm{e}^{-aE}\;, \quad (8)$$

$$\mathcal{N} = \int \mathrm{d}E\, \rho(E)\, \theta_{[E_0,\delta E]}\, \mathrm{e}^{-aE}\;, \quad (9)$$

$$\theta_{[E_0,\delta E]} = \begin{cases} 1 & \text{for} \quad E_0 \le E < E_0 + \delta E, \\ 0 & \text{elsewhere.} \end{cases} \quad (10)$$

If the energy interval is small enough, i.e., if (6) is a good approximation, we should be able to choose $a$ to compensate $a(E_0)$. This would leave us with a flat energy histogram and with

$$\langle\!\langle E\rangle\!\rangle(a) \;=\; E_0 + \frac{\delta E}{2}\;, \quad \text{for} \;\; a = a(E_0). \quad (11)$$

Assume now that $a_n$ is an approximation for $a(E_0)$ such that $x = [a(E_0) - a_n]\,\delta E \ll 1$. Defining $\Delta E := E - E_0 - \delta E/2$, we then find using (6)

$$\langle\!\langle \Delta E\rangle\!\rangle(a_n) \;=\; \frac{\delta E^2}{12}\,[a(E_0) - a_n] \;+\; \mathcal{O}(x^3\,\delta E)\;. \quad (12)$$

Ignoring the higher order correction and solving for $a(E_0)$, we obtain a better approximation $a_{n+1}$:

$$a_{n+1} \;=\; a_n \;+\; \frac{12}{\delta E^2}\,\langle\!\langle \Delta E\rangle\!\rangle(a_n)\;. \quad (13)$$

The central idea is to iterate the latter equation until

$$\langle\!\langle \Delta E\rangle\!\rangle(a_\infty) \;=\; 0 \;\;\Rightarrow\;\; a_\infty = a(E_0)\;,$$

where we have used (11). We point out that the truncated expectation values can be easily estimated by means of Monte-Carlo methods. To this aim, we insert (2) into (8) to obtain:

$$\langle\!\langle f(E)\rangle\!\rangle(a) = \frac{1}{\mathcal{N}} \int_{[E_0,\delta E]} \mathcal{D}U_\mu\; f\Big(S[U]\Big)\; \mathrm{e}^{-aS[U]}\;, \quad (14)$$

$$\mathcal{N} = \int_{[E_0,\delta E]} \mathcal{D}U_\mu\; \mathrm{e}^{-aS[U]}\;. \quad (15)$$

The subscript of the integral indicates that updates of configurations the action of which falls outside the desired energy interval are discarded. There are many Monte-Carlo techniques to estimate the truncated expectation value in (14), the Metropolis algorithm and the Heat-Bath approach being the two most obvious choices. We have tested both techniques and found that our method for estimating $a(E_0)$ is robust. The numerical results shown below have been obtained by an adapted Heat-Bath algorithm with a 100% acceptance rate (details of the algorithm will be published in a forthcoming paper).

Let us now consider the SU(2) gauge theory to illustrate our approach in practice. If $N^4$ is the number of lattice points, the maximal action is given by $E_{\max} = 6N^4$. We here consider the energy interval $I := [E_0, E_0 + \delta E] = [0.650, 0.651]\,6N^4$. The first task is to generate a lattice configuration $\{U_\mu\}$ the action of which falls into the energy interval $I$. For this purpose, we start with a "cold" configuration $U_\mu(x) = 1$, and update the configuration forcing it to reach the desired energy interval. We then pick a start value for the iteration (13), which has been $a_0 = -2$ in this preliminary study. We perform 25 energy restricted Monte-Carlo sweeps at $a_0$ (see (14)), where each sweep consists of $N^4$ updates of randomly chosen individual links.

In order to evaluate the next $a_i$ the expectation value $\langle\!\langle \Delta E\rangle\!\rangle$ is evaluated using the energy restricted Monte-Carlo method (see (14)). For this, we have used 384

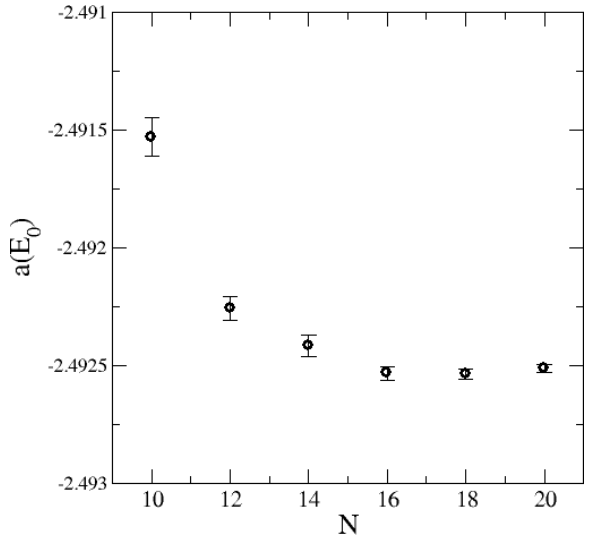


FIG. 3. The estimates for $a(E_0)$ for $E_0 = 0.650 \times 6N^4$ as a function of the lattice size.

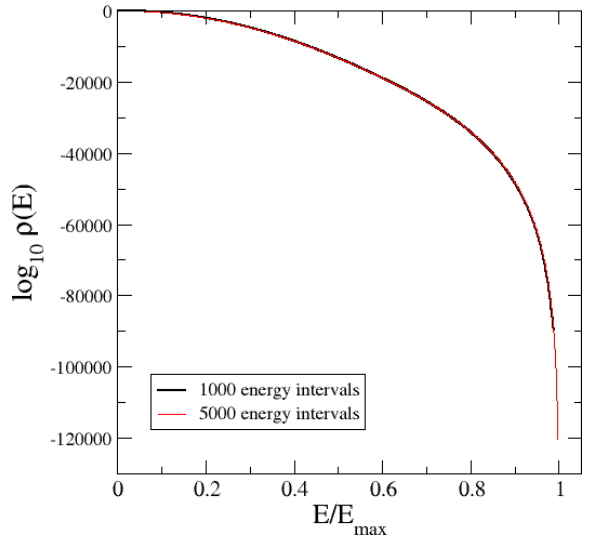


FIG. 4. The logarithm (base 10) of the density of states for the SU(2) gauge theory using a $10^4$ lattice.

measurements divided in 48 independent runs each contributing 8 Monte-Carlo sweeps (these calculation are performed on the HPC computing facilities at the Plymouth University). The corresponding estimator is then used to obtain an improved value $a_1$. This procedure is reiterated $n$ times, $n > 1$, until the value of $a$ starts to fluctuate around a central value. The thermalisation history is shown in figure 1: for small lattice sizes such as $10^4$, a thermalised state is reached after 10 iterations while for our biggest lattice $20^4$ roughly 80 iterations are necessary to reach an equilibrium. To keep control of the autocorrelation in the determination of the solution of the iterative procedure we have evaluated the integrated autocorrelation time ($\tau_{int}$) of $\langle\langle \Delta E \rangle\rangle$. In particular the measure of $\tau_{int}$ for the highest energy gap yields a value

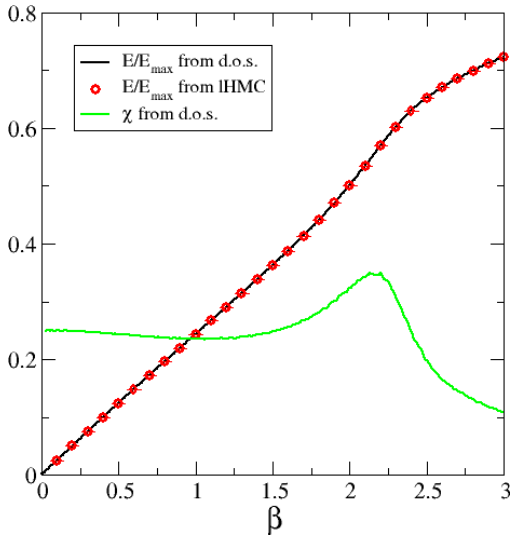


FIG. 5. Average plaquette for a SU(2) gauge theory on a $10^4$ lattice obtained by means of the density of states and local-hybrid Monte-Carlo. Also shown is the specific heat $\chi(\beta)$, Eq. (17).

always smaller that two steps for each of our volumes.

Having control of the autocorrelation time allows us to reliably define a statistical error of $\langle\langle \Delta E \rangle\rangle$ which directly feeds into the uncertainty for $a_{n+1}$ (see (13)). Rather than to spend all numerical resources to obtain a high-precision estimate for $\langle\langle \Delta E \rangle\rangle$ we found is advantageous to feed the more noisy estimator into the iteration (13) and to average the $a_n$ values of the resulting sequence. The standard error of $a_n$ for an average over a bin of 10 iterations *after* thermalisation is shown in figure 2. We roughly find that the error decreases like $1/\sqrt{V}$ where $V$ is the lattice volume. The lack of autocorrelation reflects in the good scaling of the error with the volume showing the efficiency of the algorithm also for large volumes. In particular, this observation is true even when studying energy intervals for which we would normally expect strong effects in autocorrelation due to critical slowing down (for example for $0.850 \leq E/E_{\max} \leq 0.851$ and $V = 20^4$ we find $\tau_{int} = 1.8(1)$).

For the determination of $a(E_0)$, 187 iterations have been performed for thermalisation and 312 further iterations were carried out to estimate $a(E_0)$. Our findings as a function of the lattice size are shown in figure 3.

Once $a(E_0)$ has been obtained for all energies $E_0^i = i \times \delta E$ (we here only consider positive energies), the density of states $\rho(E)$ can be easily constructed from (6):

$$\rho(E) = \prod_{i=1}^{k} \mathrm{e}^{a(E_0^i)\,\delta E} \, \exp\Big\{ a(E_0)\,(E - E_0^k) \Big\} \qquad (16)$$

for $E_0^k \leq E < E_0^{k+1}$. Thereby, we have normalised the density of states such that $\rho(E = 0) = 1$. Our numerical result is shown in figure 4. In order to estimate any influence of the discretisation error, we have calculated the

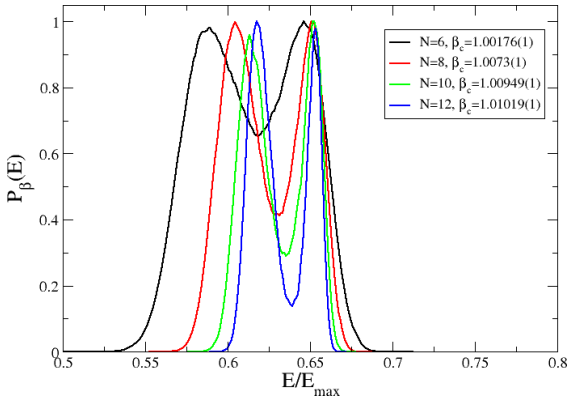


FIG. 6. The probability density $P_\beta(E)$ for a compact $U(1)$ gauge theory at critical coupling for several lattice sizes $N^4$.

density of states by splitting the energy interval $[0, E_{\max}]$ into 1000 and 5000 energy intervals. Both curves fall on top of each other in figure 4. As a proof of concept that our numerical approach does yield high precision expectation values, we have calculated the average plaquette $\langle E\rangle/E_{\max}$ using (4). As expected, only a small energy window with $a(E) \approx \beta$ significantly contributes to the expectation value. Care has been taken to handle potentially large numbers. We have compared our result with that from a standard method using local-hybrid Monte-Carlo. A very good agreement is observed. An observable which is generically difficult to estimate due to cancellations is the specific heat, which we define by

$$\chi(\beta) \;=\; \frac{1}{6N^4}\Big(\langle E^2\rangle \;-\; \langle E\rangle^2\Big), \qquad (17)$$

where the expectation values are obtained by means of (4). Our numerical findings for $\chi$ are also shown in figure 5. We have checked for a few $\beta$ values that our result agrees with that obtained by standard methods.

We have finally tested our approach for the compact U(1) gauge with Wilson action (5). Here, the links are U(1) group elements, i.e., $U_\mu(x) = \exp\{i\theta_\mu(x)\}$ with $\theta_\mu(x) = -\pi \ldots \pi$ being the dynamical degrees of freedom featuring in the functional integral with a constant measure. By means of a large scale investigation on the basis of the Borgs-Kotecky finite size scaling analysis, it has been finally established in [9] that compact U(1) possesses a weak first-order phase transition at $\beta = \beta_c \approx 1.0111331(21)$ (in the infinite volume limit). An unmistakable sign for a first order transition is the characteristic double-peak structure in the action probability density, i.e.,

$$P_\beta(E) \;=\; \rho(E)\,\exp\{\beta E\}\;, \qquad (18)$$

for $\beta \to \beta_c$. It turns out that this double-peak structure is very sensitive to variations of $\beta$ allowing a high precision determination of $\beta_c$ at finite volume, i.e., the critical coupling for which the peaks are of equal height. Note that we have normalised $P_\beta(E)$ such that its maximum value equals one. The critical couplings $\beta_c$, listed in the graph, are in good agreement with those from the large scale study [9].

In conclusions, we have developed a modified version of the Wang-Landau algorithm suitable for theories with continuous degrees of freedom. We have shown that the density of states for a SU(2) gauge theory can be calculated over a range of 120,000 orders of magnitudes even for a lattice as large as $20^4$. Our approach reliably reproduces the critical couplings of the weak first order transition of the compact U(1) gauge theory. Using the Cabibbo Marinari method [10], our approach can be generalised to SU($N_c$) Yang-Mills theories. Quantities of interests which are earmarked for our approach are thermodynamic potentials [11], vortex free energies [12] and electric fluxes for the study of the mass-gap and confinement [13]. Finally, we point out that the statistical error for expectation values obtained by the density of states method can be obtained by the bootstrap technique. A careful investigation of the statistical and possible systematic errors (from which our results seem to be free) will be reported elsewhere.

**Acknowledgments:** This work is supported by STFC under the DiRAC framework. We are grateful for the support from the HPCC Plymouth, where the numerical computations have been carried out. BL is supported by the Royal Society and by STFC.

[1] M. Creutz, Phys.Rev. **D21**, 2308 (1980).
[2] K. G. Wilson, Phys.Rev. **D10**, 2445 (1974).
[3] F. Wang and D. P. Landau, Phys. Rev. Lett. **86**, 2050 (2001).
[4] A. Hietanen and B. Lucini, Phys.Rev. **E84**, 056702 (2011).
[5] B. A. Berg and A. Bazavov, Phys.Rev. **D74**, 094502 (2006), arXiv:hep-lat/0605019 [hep-lat].
[6] B. Bringoltz and S. R. Sharpe, Phys.Rev. **D78**, 074503 (2008), arXiv:0807.1275 [hep-lat].
[7] J. Xu and H.-R. Ma, Phys.Rev. **E75**, 041115 (2007).
[8] S. Sinha and S. Kumar Roy, Phys.Lett. **A373**, 308 (2009).
[9] G. Arnold, B. Bunk, T. Lippert, and K. Schilling, Nucl.Phys.Proc.Suppl. **119**, 864 (2003), arXiv:hep-lat/0210010 [hep-lat].
[10] N. Cabibbo and E. Marinari, Phys.Lett. **B119**, 387 (1982).
[11] L. Giusti and H. B. Meyer, JHEP **1111**, 087 (2011), arXiv:1110.3136 [hep-lat].
[12] T. G. Kovacs and E. Tomboulis, Phys.Rev.Lett. **85**, 704 (2000), arXiv:hep-lat/0002004 [hep-lat].
[13] P. de Forcrand and L. von Smekal, Phys.Rev. **D66**, 011504 (2002), arXiv:hep-lat/0107018 [hep-lat].