Density of States in Gauge Theories

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The density of states is calculated for the SU(2), SU(3), and a compact U(1) lattice gauge theories 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).

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Monte Carlo simulations of theories discretized on a Euclidean space-time lattice 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. This strategy is successful for computations of observables that can be expressed as a vacuum expectation value (VEV) on a theory with a semipositive definite path integral measure. However, 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 semipositive (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 β the inverse coupling. For this theory, the path integral in Euclidean space-time is given by

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

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

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

the VEV of an observable $O(E)$ becomes

$$\langle O \rangle = \frac{1}{Z} \int \rho(E) O(E) e^{\beta E} dE, \quad Z = \int \rho(E) e^{\beta E} dE. \tag{3}$$

If the density of states is known, $\langle O \rangle$ can be obtained by means of standard integration.

The density of states has been previously explored for a U(1) and SU(2) gauge theory using respectively multicanonical [1] and canonical [2] methods. For systems with discrete energy levels, an efficient algorithm for computing $\rho(E)$ has been proposed by Wang and Landau in Ref. [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., Ref. [4] for a recent example). Despite its popularity in statistical mechanics, the Wang-Landau algorithm has found only limited applications in lattice gauge theory [5–7] (An earlier attempt to measure the density of states is reported in [8].). In fact, an efficient algorithm for sampling the density of states of continuous systems along the lines of Ref. [3] is not available to date. In this Letter, 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 Letter we adopt the lattice regularization, which leaves us with a N^4 cubic lattice as the discretization 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.,

$$S[U] = \sum_{\mu > \nu, x} \frac{1}{N_c} \mathrm{Re\,tr}[U_\mu(x) U_\nu(x+\mu) U_\mu^\dagger(x+\nu) U_\nu^\dagger(x)], \tag{4}$$

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

$$\rho(E) = \rho(E_0) \exp\{a(E_0)(E - E_0)\} \tag{5}$$

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:

$$a(E_0) = \frac{d\ln\rho(E)}{dE}\bigg|_{E=E_0}. \quad (6)$$

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

$$\langle\langle f(E)\rangle\rangle(a) = \frac{1}{\mathcal{N}}\int dE f(E)\rho(E)\theta_{[E_0,\delta E]}e^{-aE}, \quad (7)$$

$$\mathcal{N} = \int dE\rho(E)\theta_{[E_0,\delta E]}e^{-aE}, \quad (8)$$

$$\theta_{[E_0,\delta E]} = \begin{cases} 1 & \text{for } E_0 \le E < E_0 + \delta E. \\ 0 & \text{elsewhere.} \end{cases} \quad (9)$$

If the energy interval is small enough, i.e., if (5) 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

$$\langle\langle E\rangle\rangle(a) = E_0 + \frac{\delta E}{2}, \qquad \text{for } a = a(E_0). \quad (10)$$

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 (5)

$$\langle\langle \Delta E\rangle\rangle(a_n) = \frac{\delta E^2}{12}[a(E_0) - a_n] + \mathcal{O}(x^3\delta E). \quad (11)$$

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

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

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 (10). 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 (7) to obtain:

$$\langle\langle f(E)\rangle\rangle(a) = \frac{1}{\mathcal{N}}\int_{[E_0,\delta E]}\mathcal{D}U_\mu f(S[U])e^{-aS[U]}, \quad (13)$$

$$\mathcal{N} = \int_{[E_0,\delta E]}\mathcal{D}U_\mu e^{-aS[U]}. \quad (14)$$

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 (13), 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 elsewhere).

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 (12), which has been $a_0 = -2$ in this preliminary study. We perform 25 energy restricted Monte Carlo sweeps at a_0 [see (13)], 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 (13)]. For this, we have used 384 measurements divided in 48 independent runs each contributing 8 Monte Carlo sweeps. 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 thermalization history is shown in Fig. 1: for small lattice sizes such as 10^4, a thermalized 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 (τ_{int}) of $\langle\langle \Delta E\rangle\rangle$. In particular the measure of τ_{int} for the highest energy gap yields a value always smaller than two steps for each of our volumes.

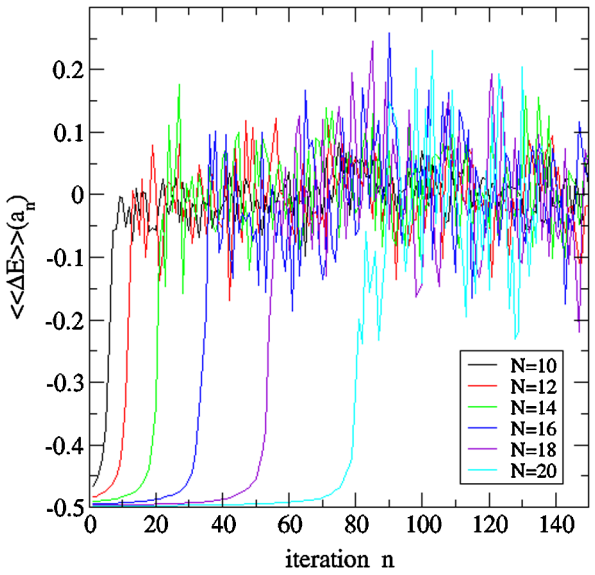

FIG. 1 (color online). The thermalization history for a SU(2) gauge theory for lattice sizes $10^4 \ldots 20^4$.

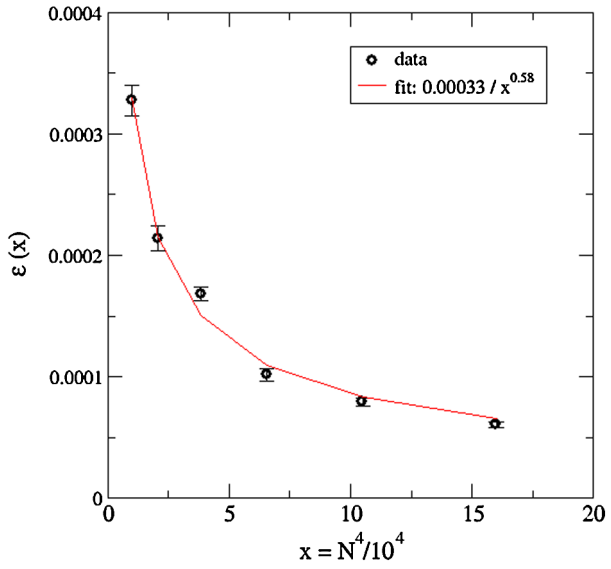

FIG. 2 (color online). The statistical error for the estimate of $a(E_0)$ for lattice sizes $10^4 \ldots 20^4$.

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 (12)]. Rather than spending all numerical resources to obtain a high precision estimate for $\langle\langle \Delta E \rangle\rangle$ we found it advantageous to feed the more noisy estimator into the iteration (12) 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 thermalization is shown in Fig. 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 $0.850 \leq E/E_{\text{max}} \leq 0.851$ and $V = 20^4$ we find $\tau_{\text{int}} = 1.8(1)$].

For the determination of $a(E_0)$, 187 iterations have been performed for thermalization and 312 further iterations were carried out to estimate $a(E_0)$. Our findings as a function of the lattice size are shown in Fig. 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 (5):

$$\rho(E) = \prod_{i=1}^{k} e^{a(E_0^i)\delta E} \exp\{a(E_0)(E - E_0^k)\}, \qquad (15)$$

for $E_0^k \leq E < E_0^{k+1}$. Thereby, we have normalized the density of states such that $\rho(E = 0) = 1$. Our numerical result is shown in Fig. 4. In order to estimate any influence of the discretization error, we have calculated the density of states by splitting the energy interval $[0, E_{\text{max}}]$ into 1000 and 5000 energy intervals. Both curves fall on top of each other in Fig. 4. We also show the corresponding result for the SU(3) gauge theory. As a proof of concept that our numerical approach does yield high precision expectation values, we have calculated the average plaquette $\langle E \rangle / E_{\text{max}}$ using (3). 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 calculations. 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

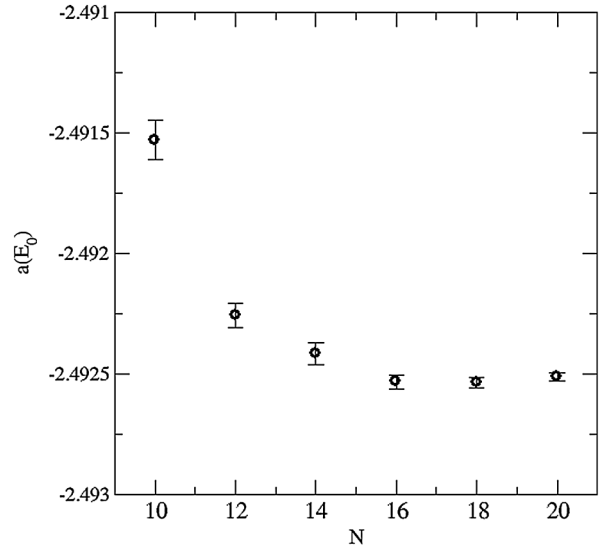

FIG. 3. The estimates for $a(E_0)$ for $E_0 = 0.650 \times 6N^4$ as a function of the lattice size.

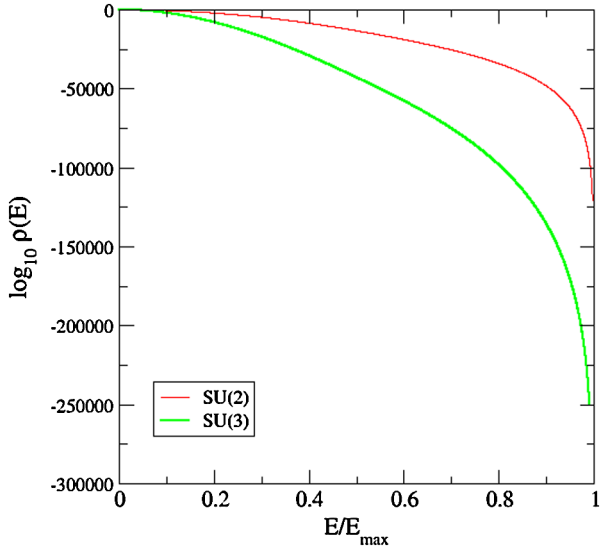

FIG. 4 (color online). The logarithm (base 10) of the density of states for the SU(2) and SU(3) gauge theories using a 10^4 lattice.

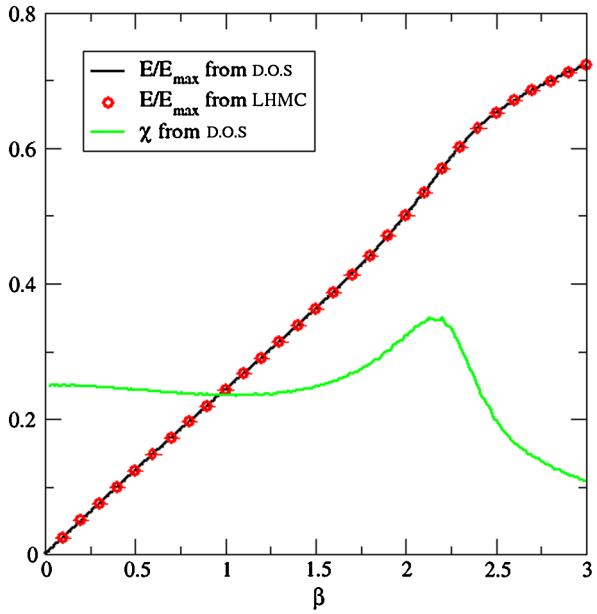

FIG. 5 (color online). Average plaquette for a SU(2) gauge theory on a 10^4 lattice obtained by means of the density of states and localized hybrid Monte Carlo (LHMC) calculation. Also shown is the specific heat $\chi(\beta)$.

$\chi(\beta) = (\langle E^2\rangle - \langle E\rangle^2)/6N^4$, where the expectation values are obtained by means of (3). Our numerical findings for χ are also shown in Fig. 5. We have checked for a few β values that our result agrees with that obtained by standard methods.

We have finally tested our approach for the compact U(1) gauge theory 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 Ref. [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., $P_\beta(E) = \rho(E)\exp\{\beta E\}$, for $\beta \to \beta_c$. It turns out that this double-peak structure is very sensitive to variations of β allowing a high precision determination of β_c at finite volume, i.e., the critical coupling for which the peaks are of equal height. Note that we have normalized $P_\beta(E)$ such that its maximum value equals one. The critical couplings β_c, listed in the graph in Fig. 6, are in good agreement with those of Ref. [9].

In conclusion, 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 magnitude even

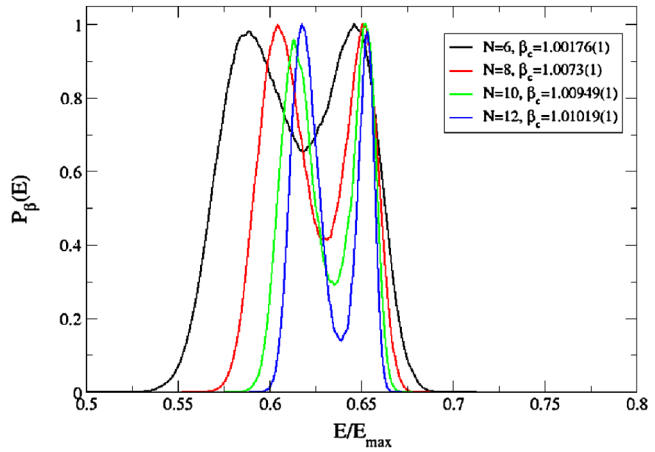

FIG. 6 (color online). The probability density $P_\beta(E)$ for a compact $U(1)$ gauge theory at critical coupling for several lattice sizes N^4.

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. A careful investigation of the statistical and possible systematic errors (from which our results seem to be free) will be reported elsewhere. Using the Cabibbo-Marinari method, our approach can be generalized to SU(N_c) Yang-Mills theories. Quantities of interest which are earmarked for our approach are thermodynamic potentials [10], vortex free energies [11], and electric fluxes for the study of the mass gap and confinement [12]. Work is in progress for generalizing the present method to deal with complex action systems, with the view of using it in finite density QCD.

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Note added.—After this Letter was published, we learned of Ref. [13], where a similar strategy was investigated for discrete spin systems.

[1] A. Bazavov, B. Berg, D. Du, and Y. Meurice, Phys. Rev. D **85**, 056010 (2012).
[2] A. Denbleyker, D. Du, Y. Liu, Y. Meurice, and A. Velytsky, Phys. Rev. D **78**, 054503 (2008).
[3] F. Wang and D. P. Landau, Phys. Rev. Lett. **86**, 2050 (2001).
[4] A. Hietanen and B. Lucini, Phys. Rev. E **84**, 056702 (2011).
[5] B. A. Berg and A. Bazavov, Phys. Rev. D **74**, 094502 (2006).
[6] B. Bringoltz and S. R. Sharpe, Phys. Rev. D **78**, 074503 (2008).
[7] W. Unger and P. de Forcrand, arXiv:1111.1434.

[8] V. Azcoiti, G. Di Carlo, and A. F. Grillo, Phys. Rev. Lett. **65**, 2239 (1990).
[9] G. Arnold, B. Bunk, T. Lippert, and K. Schilling, Nucl. Phys. B, Proc. Suppl. **119**, 864 (2003).
[10] L. Giusti and H. B. Meyer, J. High Energy Phys. 11 (2011), 087.
[11] T. G. Kovacs and E. T. Tomboulis, Phys. Rev. Lett. **85**, 704 (2000).
[12] P. de Forcrand and L. von Smekal, Phys. Rev. D **66**, 011504 (2002).
[13] J. Viana Lopes, M. D. Costa, J. M. B. Lopes dos Santos, and R. Toral, Phys. Rev. E **74**, 046702 (2006).