Nonextensive lattice gauge theories: algorithms and methods

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Abstract

High-energy phenomena presenting strong dynamical correlations, long-range interactions and microscopic memory effects are well described by nonextensive versions of the canonical Boltzmann-Gibbs statistical mechanics. After a brief theoretical review, we introduce a class of generalized heat-bath algorithms that enable Monte Carlo lattice simulations of gauge fields on the nonextensive statistical ensemble of Tsallis. The algorithmic performance is evaluated as a function of the Tsallis parameter $q$ in equilibrium and nonequilibrium setups. Then, we revisit short-time dynamic techniques, which in contrast to usual simulations in equilibrium present negligible finite-size effects and no critical slowing down. As an application, we investigate the short-time critical behaviour of the nonextensive hot Yang-Mills theory at $q$-values obtained from heavy-ion collision experiments. Our results imply that, when the equivalence of statistical ensembles is obeyed, the long-standing universality arguments relating gauge theories and spin systems hold also for the nonextensive framework.

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1. Introduction

There is increasing evidence that generalizations of the canonical thermostatistics of Boltzmann-Gibbs (BG) are useful to describe important phenomenological aspects of relativistic hadronic collisions [1, 2]. Traditionally, a QCD inspired formula à la Hagedorn [3] is employed to fit the cross sections ($\sigma$) of hadrons as a function of their transverse momenta ($p_T$)

$$E \frac{d^3\sigma}{dp} = C \cdot \left( 1 + \frac{p_T}{p_0} \right)^{-\alpha} \rightarrow \begin{cases} p_T \rightarrow 0 \Rightarrow \exp\left( -\frac{\alpha p_T}{p_0} \right) \\ p_T \rightarrow \infty \Rightarrow \left( \frac{p_T}{p_0} \right)^{\alpha} \end{cases}$$ (1)

with parameters $C$, $p_0$ and $\alpha$. Where the mean transverse momentum of the system $\langle p_T \rangle$ is related to its hadronization temperature $T$ in equilibrium.

However, such temperature shall naturally fluctuate among events [4], in a clear far-from-equilibrium scenario. Therefore, the usual BG picture shall be generalized to naturally accommodate such fluctuations, this is done by considering a Tsallis [5, 6] distribution

$$E \frac{d^3\sigma}{dp} = C_q \cdot \left[ 1 - (1 - q) \frac{p_T}{p_0} \right]^{\frac{1}{q-1}}.$$ (2)

Here $\alpha = \frac{1}{q-1}$, $p_0 = \frac{T}{q-1}$ and $C_q$ is a normalization, whereas the nonextensive parameter $q$ is related to the variance of $T$ by

$$q = 1 + \frac{Var(T)}{\langle T \rangle^2}. \quad (3)$$

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Along the last years variations of the approach in Eq. (2) have been verified by different collaborations, as ALICE [8], ATLAS [9] and CMS [10] at LHC and PHENIX [11] and STAR [12] at RHIC, which has fit experimental data by power-like (Levy) distributions using Tsallis formulae [13, 14].

While equations Eq. (1) and Eq. (2) may seem similar from the mathematical point, their underlying physics is quite distinct. The nonextensive expression admits a complex (steady state) thermal equilibrium for any $p_T$, which can be described by just two parameters $T$ and $q$. Thus, it is an unifying statistical mechanics approach that does not rely on any particular model, or theoretical regime of a more fundamental theory (i.e. perturbative vs nonperturbative QCD) [2], to be derived from.

Still, this conceptual difference plays a central role when modeling heavy-ion collisions through a hydrodynamical approach with evolution [15]. There, the transverse momentum distributions of multiple particle species is usually described by a Boltzmann-Gibbs Blast-Wave (BGBW) model, see [16] (and references therein). This brings most of physical insights about the behaviour of the fireball. Nevertheless, such an equilibrium description is believed to break at high $p_T$, when nonequilibrium effects and hard processes will exhibit power-law tail [7]. So, generalizations of BGBW incorporating principles of Tsallis thermostatistics [16] are necessary (TBW), and in fact they have shown to be powerful enough to describe experimental data [1, 11, 17].

While nonextensive extensions of well-known phenomenological models is an attractive area, with potential implications [18] – see also [19] for q-Walecka and [20] for q-NJL — their derivation from first principles is not fully understood yet [21, 22]. Therefore, it is of high theoretical interest to generalize first-principle nonperturbative methods, as the lattice formalism of nonabelian gauge theories [23], to the Tsallis ensemble. Moreover, from a pure computational perspective, lattice simulations may benefit from Tsallis weight, hence it enhances the tunneling rate among metastable states during phase transitions [24].

In this context, following the generalized master equation approach of [25], we introduce a generalized hybrid heat-bath algorithm to enable Monte Carlo simulations of lattice Yang-Mills (YM) theory in the Tsallis ensemble. In addition, this algorithm can be also easily adapted to other $SU(N)$ gauge theories. Thus, we perform a rigorous analysis of algorithmic performance in 2d lattices, where the $SU(2)$ theory is exactly solvable. This solution helps on evaluating integrated correlation-times of critical plaquettes, as a function of the lattice-side and $q$, while investigating a region of constant physics [26]. In agreement with previous studies [24, 27] we observe that setups with $q > 1$ induce significant improvements on computational efficiency when compared to the canonical case ($q = 1$).

On the other hand, when considering finite-temperature simulations on equilibrium, universality has been a cornerstone principle to understand the thermodynamics of gauge theories in the canonical ensemble. For instance, even dynamical aspects of such theories, as their screening-mass spectra [28], were predicted from condensed-matter analogous. Also, based on arguments of symmetry, QCD with two dynamic quarks undergoes a phase transition with universal critical scaling in the class of the 3d $O(4)$ continuous-spin mode [29]. Furthermore, there is the long-standing argument by Svetitsky and Yaffe [30] relating critical quenched $SU(N)$ gauge fields in $d + 1$ dimensions to $Z_N$ spin systems in $d$–dim.

Those simulations are challenging, not only because finite-size (FS) effects — and their necessary scaling extrapolations — have to be keep under control, but also because the well-know critical slowing down (CSD) effect [31]. This implies exponentially diverging correlation times of observables, and so their statistical errors. A way to alleviate that computational burden comes from short-time dynamical simulations, for a review see [32, 33]. This technique allows for extracting the critical behaviour, summarized in a set of dynamic and static exponents, of spin-systems or gauge fields without appreciable FS or CSD effects. This feature is rooted on the findings [34] that even during a short-time transient regime, before (Monte Carlo) equilibration happens, the hamiltonian dynamics already exhibits universal scaling.

\footnote{Incidentally, this spin system can be simulated using a heat-bath algorithm shared by lattice Y.M. theory [26].}
Considering that few is known about the aforementioned critical properties of nonextensive gauge theories, we investigate through short-time simulations the finite-temperature 3d SU(2) lattice Y.M. theory \( (YM^{3d}_2) \) in the Tsallis ensemble. Despite of being considerably simpler than unquenched QCD, the \( YM^{3d}_2 \) theory is nontrivial. Actually, it has been shown to be a good theoretical model for understanding fundamental properties of confinement. Concerning gluonic Wilson action \( Y M \) propagators, no relevant discrepancies to QCD were found at gauge groups \( 35 \) or dimensionality \( 30 \) levels. In addition, around criticality \( YM^{3d}_2 \) is related to the bidimensional Ising model, an exactly solvable system, which turns that gauge theory more auspicious for high-precision comparative studies.

As a matter of fact, we have focused our simulations on values of the nonextensive parameter \( q \approx 1 \) — as a perturbation around BG thermodynamics — and \( q = 1.10 \), a value favoured by experimental data fits \([1, 2, 13]\). We have observed that for \( q \approx 1 \) small deviations from usual BG behaviour are seen. While in the \( q > 1 \) regime the temperature of the phase-transition is monotonically increased with \( q \) (i.e. \( T_{q>1} > T_{q=1} \)), as theoretically expected \([2, 7]\). Besides that, by performing a Binder cumulant analysis (in equilibrium) \([37]\) we confirm that our results are not afflicted by any FS effect. More interestingly, not only the static and dynamic exponents of the nonextensive theory, but also its universal cumulant values, can be explained by (and generalizes) universality arguments \([30]\).

The article is organized as follows: in Section 2 the nonextensive thermostatistics of Tsallis is outlined. Its connections with the usual Boltzmann-Gibbs statistics are discussed in the sense of superstatistics, and finally, applications to gauge theories are provided. The Section 3 reviews short-time dynamic simulation techniques for gauge theories. It gives an outlook on how to overcome the critical slowing down phenomena, while evaluating static and dynamic exponents. Our generalized algorithmic proposal is presented in Section 4, after briefly reviewing the theory of Markov processes and (generalized) detailed balance. The necessary modifications to usual heat-bath updating engines \([26]\) is theoretically motivated and implemented. In Section 5, numerical results on algorithmic performance are analysed for the 2d SU(2) gauge theory and, the nonextensive relaxation dynamics for finite-temperature 3d SU(2) theory is studied. Main conclusions and prospective research directions are the focus of Section 6.

2. Nonextensive thermostatistics of lattice gauge theories

The lattice gauge theory formalism allows for \textit{ab initio} thermodynamic analysis of quantum fields at finite-temperature nonperturbative regimes \([23]\). Most times it is performed in the quenched approximation, where quark-loop effects are neglected. Within this approach the deconfinement phase transition of SU\((N)\) theories can be related by universality arguments to the magnetic transition of \( Z_N \) spin models \([30]\).

A realization for pure gauge SU\((N)\) theories in \( d \)-dimensional lattices is given \([23]\) by the Wilson action

\[
SW [U] \equiv \beta \sum_x \sum_{\mu,\nu=1}^d \left\{ 1 - \frac{1}{N} Re(TrP_{\mu\nu}) \right\}, 
\]

where gauge links \( U_\mu (x) \in SU(N) \) are combined to build a gauge-invariant plaquette

\[
P_{\mu\nu} \equiv U_\mu (x) U_\nu (x + \hat{\mu} a) U_{\mu}^{-1} (x + \hat{\nu} a) U_{\nu}^{-1} (x). 
\]

The lattice-coupling \( \beta = 2N/g_s^2 a^{d-2} \) is set in terms of the gauge-field coupling \( g_s \) and the physical lattice spacing \( a \).

In the canonical ensemble the temperature of equilibrium is identified with the inverse length of the temporal direction (i.e. \( T^{-1} = aL_t \)) of an assymetric lattice, whose volume is \( V = a^d L_x^{d-1} L_t \) \([23]\). Thus, thermal expectation values of any gauge-invariant operator \( \mathcal{O} \) may be computed by

\[
\langle \mathcal{O} \rangle_{BG} = \frac{\sum_U \mathcal{O} (U) e^{-SW(U)} }{\sum_U e^{-SW(U)}}. 
\]
Among such observables is the (spatially averaged) Polyakov loop $\bar{W} \equiv \langle W(x,y,z) \rangle = \langle Tr \prod_{n=1}^{n=L} U_t(x,y,z,an) \rangle$, the order parameter of deconfinement phase transition.

Tsallis introduced a nonextensive generalization of the usual canonical ensemble $[5]$ by postulating a pseudo-additive entropy

$$S_q = \frac{(1 - Tr \hat{\rho})}{q - 1}. \quad (7)$$

Here, the real-number $q$ (Tsallis parameter) regulates the degree of non-additivity of the generalized entropy $S_q^{A+B} = S_q^A + S_q^B + (1 - q)S_q^A S_q^B$, and $\hat{\rho}$ is a density operator. The explicit form of $\hat{\rho}$ is obtained by a constrained maximization of $S_q$ $[6, 38, 39]$ which, for instance, leads to

$$\hat{\rho} = Z_q^{-1} e^{-H/T} = Z_q^{-1} \left[ 1 - (1 - q) \frac{\hat{H}}{T} \right]^{1/(1-q)}. \quad (8)$$

Where $Z_q$ stands for the $q$--dependent partition function of Tsallis (i.e. a normalization factor) and $\hat{H}$ is the Hamiltonian of the system at physical temperature $T$.

The resulting Tsallis statistics is also known to be a particular case of superstatistics $[40]$, derived as a superposition of different BG statistics, with special relevance for nonequilibrium systems. Thereby, the Tsallis weight $\omega_k$ can be obtained from a (Gamma) integral-transform over Boltzmann-Gibbs weights

$$\omega_k = \frac{1}{Z_q} \int_0^\infty d\theta w_c(\theta) e^{-\theta \beta E_k}, \quad (9)$$

where $q = 1 + 1/c$ and $w_c(\theta) = \frac{c^c}{\Gamma(c)} \theta^{c-1} e^{-\theta}$. Thus, any BG expectation value can be converted into a Tsallis one if it is known as a function of $\beta$. In particular, the respective partition functions of Boltzmann-Gibbs ($Z_{BG}$) and of Tsallis ($Z_T$) are related by

$$Z_T(\beta) = \sum_k \int_0^\infty d\theta w_c(\theta) e^{-\theta \beta E_k} = \int_0^\infty d\theta w_c(\theta) Z_{BG}(\theta \beta). \quad (10)$$

Considering the case of pure gauge theories, where $Z_{BG} = \int DU e^{-S_W(U)}$, the expression in Eq. (10) is explicitly written as

$$Z_T = \frac{c^c}{\Gamma(c)} \int_0^\infty d\theta e^{-\theta} \theta^{c-1} \int DU e^{-S_{W,\beta}(U)}, \quad (11)$$

where $S_{W,\beta}(U)$ is the usual Wilson action of Eq.$[4]$ evaluated$[2]$ for $\hat{\beta} = \theta \beta$. Then, by assuming a finite $c$, the $\theta$--integration and the path-integral can be exchanged

$$Z_T = \int DU \frac{c^c}{\Gamma(c)} \int_0^\infty d\theta e^{-\theta} \theta^{c-1} e^{-S_{W,\beta}(U)} \rightarrow Z_q = \int DU e^{-S_W(U)}. \quad (12)$$

Therefore, once the Tsallis formalism reduces to the usual BG approach in the limit $q = 1$ (i.e. $S_q = S_{BG} = -Tr \ln \hat{\rho}$) $[12, 22]$, a $q$--expectation value $\langle \cdot \rangle_q$ that generalizes Eq.$[5]$ may be written $[22, 39]$ as

$$\langle \mathcal{O} \rangle_q = \frac{\sum_U \mathcal{O}(U) e^{-S_{W}(U)}}{\sum_U e^{-S_{W}(U)}}. \quad (13)$$

\[2\]In $[41]$ (and references therein) it was shown that, for systems with constant total energy, volume fluctuations are equivalent to temperature fluctuations. In fact, both these (Gamma) fluctuations can equivalently lead to the Tsallis form of the respective distributions for energy spectra. Thus, it is quite natural to employ a symmetric lattice-coupling $\beta$ (i.e. the same $\beta$) for space and “time” directions in the Wilson action.
3. Short-time critical dynamics

Renormalization group techniques predict \cite{34} that after a sudden quench to the critical temperature $T_c$ many physical systems can display universal dynamical behaviour even during the early (nonequilibrium) evolution times. Curiously, along this transient process finite-size effects and critical slowing down phenomena \cite{31} are almost absent. This may be understood by realizing that in such simulations observables are averaged over time-slices from independent Markov chains, which are started from similar initial states \cite{37}.

Thence, this technique allows for efficient characterization of critical properties of systems undergoing relaxation to thermal equilibrium. For instance, correlation scales and critical exponents may be extracted by studying the dynamic evolution of appropriate functions of the order parameters. In particular, the order parameter for gauge theories is the so-called Polyakov loop $(W_r)$, which seems an effective magnetization $M$ of spin systems \cite{33}. Its (time-dependent) definition is given by

$$M(t) = \left\langle \frac{1}{L_s^{d-1}} \sum_{r} W_r[t] \right\rangle_{\text{samples}},$$

where $\langle \cdots \rangle_{\text{samples}}$ denotes averaging over configurations at the same Monte Carlo instant $[t]$.

When considering the dynamic relaxation from a completely ordered state, i.e. with initial magnetization $m_0 = 1$, a general scaling form for the $k$-th moment of the magnetization $M$ emerges

$$M^{(k)}(t, \tau, L_s) = b^{-k\beta/\nu} M^{(k)}(b^{-z} t, b^{1/\nu} \tau, b^{-1} L_s).$$

Here $t$ is the MC time of the dynamic relaxation, $\tau$ is the reduced coupling constant, $b$ is a rescaling factor, $\beta/\nu$ is the ratio between two (static) critical exponents, $z$ is a dynamic exponent and $L_s$ is the lattice side. This scaling form has been shown to be valid in the short-time regime for a number of different physical systems including gauge theories \cite{33,42}.

By choosing $b = t^{1/z}$ as the rescaling factor in Eq. (15) and assuring that $\tau = 0$, it leads to a power-law behaviour for the magnetization (i.e. $k = 1$) given by

$$M(t) \sim t^{-\beta/\nu z}.$$

In addition, the scaling of the cumulant

$$U = \frac{M^2(t)}{M(t)^2} - 1,$$

can be expressed \cite{42} in terms of the space dimension $d$ as

$$U(t) \sim t^{d/z},$$

thus providing the value of $z$ while fixing the ratio $\beta/\nu$.

Furthermore, at the critical line the autocorrelation of the order parameter

$$A(t) = \left\langle \frac{1}{L_s^{2(d-1)}} \sum_{r} W_r[t] W_r[0] \right\rangle_{\text{samples}},$$

also obeys a power law $A(t) \sim t^{-\eta/2z}$, while in the low temperature phase it is described by the ansatz

$$A(t) \sim t^{-\eta/2z} \exp (-t/\xi_t).$$

Where the nonequilibrium autocorrelation time $\xi_t$ is related to the equilibrium autocorrelation length $\xi_s$ through $\xi_t \propto \xi_s^d$ \cite{43}.

\footnote{It is worth to mention that when considering spin systems this relation is valid for the high-temperature phase, as explained by universal mappings described in \cite{38}.}
4. A generalized heat-bath algorithm for the Tsallis ensemble

Dynamical Monte Carlo simulations use Markov chains designed to generate, when in equilibrium, a desired target probability distribution \( P(E) \). To ensure this, a sufficient condition is known to be the detailed balance

\[
\omega[g \rightarrow g'] P[E(g)] - \omega[g' \rightarrow g] P[E(g')] = 0. \tag{21}
\]

Where, \( \omega[g' \rightarrow g] \) is the transition-rate of the system configuration from \( g \) to \( g' \), and \( E(g) \) \( E(g') \) is the energy — or alternatively, the action \( S'(g) \) — of the system before [after] the transition \( \tag{23} \).

Different updating algorithms implement Eq.\( (21) \) by constructing particular transition rules. For instance, a new configuration \( g' \) can be proposed to replace \( g \) with an \textit{a priori} selection probability \( p_{T,g}(g') \) \( \tag{41} \). After that, the proposal may be accepted with a given conditional probability \( P_A \) satisfying Eq.\( (21) \). A realization of this last step is given by the general Metropolis choice

\[
P_A = \min \left\{ 1, \frac{p_{T,g}(g) \times P[E(g')]}{p_{T,g}(g') \times P[E(g)]} \right\}. \tag{22}
\]

In particular, when \( p_{T,g}(g') = p_{T,g}(g) \) — and \( P(E) \) satisfies the BG statistics — the acceptance on Eq.\( (22) \) reduces to the well-known Metropolis criterion

\[
\omega[g \rightarrow g'] = \min\left\{ 1, \exp[-\beta(E(g') - E(g))] \right\}. \tag{23}
\]

Alternatively, for local actions, one can choose \( g' \) with probability \( p_{T,g}(g') \propto \exp[-\beta E(g')] \) to obtain the heat-bath algorithm \( \tag{44} \), whose \( P_A = 1 \).

Fortunately, for pure \( SU(2) \) gauge theories, the Wilson action Eq.\( (41) \) enables an exact implementation of the heat-bath algorithm — i.e., by taking \( p_{T,U_{\mu}}(U_{\mu}^{new}) \propto \exp[-S_{1-link}(U_{\mu}^{new})] \) — since \( S_W \) can be expressed as a sum of single-link (local) actions

\[
S_{1-link} = -\frac{\beta}{2} Tr[U_{\mu}(x)H_{\mu}(x)]. \tag{24}
\]

Here the gauge link \( U_{\mu}(x) \in SU(2) \), \( H_{\mu}(x) \) is the sum of neighbour staples written as \( H_{\mu}(x) = N_{\mu}(x)\tilde{H}_{\mu}(x) \), with \( \tilde{H}_{\mu}(x) \in SU(2) \) and \( N_{\mu}(x) = \sqrt{\det H_{\mu}(x)} \).

Then, by imposing over Eq.\( (24) \) the invariance of group measure one obtains \( \tag{26,43} \) the update step

\[
U_{\mu}(x) \rightarrow U_{\mu}^{new}(x) = V\tilde{H}_{\mu}^{-1}. \tag{25}
\]

Where the unimodular evolution matrix \( V = v_{0}I + i\vec{v} \cdot \vec{\sigma} \in SU(2) \) is generated by randomly taking \( v_{0} \) according to the distribution

\[
P(v_{0}) \propto \sqrt{1-v_{0}^2} \exp(\beta N v_{0}) dv_{0}, \tag{26}
\]

while the components of \( \vec{v} \) are isotropically chosen from \( \mathbb{R}^3 \).

An implementation of Eq.\( (26) \) was originally proposed by Creutz \( \tag{45} \), it consists on directly sampling \( v_{0} \) with probability \( P(v_{0}) \sim \exp(\beta N v_{0}) \) and so correcting for the \( \sqrt{1-v_{0}^2} \) factor by rejection. Besides that, once invariance under group measure does not constrain the vectorial part of the evolution matrix \( V \), a microcanonical overrelaxation step \( \tag{26} \) may be incorporated by taking \( \vec{v} \rightarrow -\text{sgn}(\vec{v} \cdot \vec{w})\vec{v} \), with \( W = v_{0}I + i\vec{w} \cdot \vec{\sigma} = U_{\mu}^{old}(x)\tilde{H}_{\mu}(x) \) where \text{sgn} denotes the sign function. Still, this algorithm (MHB \( \tag{26} \)) can be iteratively applied for the \( SU(2) \) subgroups of \( SU(N) \), so producing a pseudo heat-bath approach for any quenched lattice gauge theory \( \tag{22} \).

However, in a more general context, as to simulate gauge theories in the nonextensive ensemble of Tsallis, the target probabilities \( P(E) \) in Eq.\( (21) \) will become a \( q \)-generalized statistical distributions \( P_q(E) \) \( \tag{29} \). As discussed in \( \tag{25} \), in this case the usual Metropolis updating scheme in Eq.\( (23) \) becomes nonlocal even for local actions. It comes from the fact that \( q \)-exponential functions are non-additive, so single-link modifications introduce changes in the system energy that is spread all over the lattice.
To circumvent such additional computational burden one would need to devise a way to retrieve locality in the Monte Carlo updates. This can be accomplished by algorithms derived from a q-generalized detailed balance condition (see for details \cite{25}, and references therein) written\footnote{For the particular definition of \( P_q(E) \) in \cite{24}, employing escort probabilities as prescribed by TMP convention \cite{39}, one has to use slightly different definitions for q–operators. On the other hand, we employ TO convention for \( P_q(E) \) without need to escort probabilities.} as

\[
\omega [g \rightarrow g'] \otimes_q P_q [E(g)] \otimes_q \omega [g' \rightarrow g] \otimes_q P_q [E(g')] = 0. \tag{27}
\]

Where use is made of the so-called\footnote{Hence the probability density \( P_q(v_0) \) can be generated by rejection from \( p_q(v_0) \sim exp_q (\beta N v_0) \), one shall obtain \( p_q(v_0) \) by the transform method \cite{10}. For instance, \( x \) is randomly drawn following a general distribution as \( p_q(x) \sim exp_q(c \cdot x) \) by computing \( x = -q' \ln_{q'} (U) / c \), whereas the random \( U \in (0, 1) \), while \( q' = (2 - q)^{-1} \) and \( \ln_{q'} (U) = (U^{1-q'} - 1) / (1 - q') \).} algebraic q-operators

\[
a \otimes_q b = a + b + (1 - q) ab, \tag{28}
\]

\[
a \otimes_q b = \frac{a-b}{1+(1-q)b}, \tag{29}
\]

\[
a \otimes_q b = (a^{1-q} + b^{1-q} - 1)^{1/(1-q)}, \tag{30}
\]

\[
a \otimes_q b = (a^{1-q} - b^{1-q} + 1)^{1/(1-q)}. \tag{31}
\]

Which recovers the additive property of the argument \( \exp_q(a) \exp_q(b) = \exp_q(a \otimes_q b) \) as well as \( \exp_q(a) / \exp_q(b) = \exp_q(a \otimes_q b) \) while \( \exp_q(a) \otimes_q \exp_q(b) = \exp_q(a + b) \) and \( \exp_q(a) \otimes_q \exp_q(b) = \exp_q(a - b) \).

An immediate solution of Eq.\eqref{27}, for systems with local actions, was given in \cite{25} as a generalized Metropolis algorithm (q-Metropolis)

\[
\omega [g \rightarrow g'] = \min \{1, \exp_q (-\beta(E(g') - E(g)))\}, \tag{32}
\]

whose transitions depend only on the energy difference between the updated site and its neighbours.

Besides that, when considering pure gauge theories, another natural solution for Eq.\eqref{27} is a q-generalized heat-bath algorithm (q-MHB) with a priori probabilities given by \( pr_{T,U_v} (U^{\text{new}}_{\mu}) \propto \exp_q [-S_{1-\text{link}}(U^{\text{new}}_{\mu})] \). This algorithm satisfies a generalization (with q-operators) of Eq.\eqref{22} derivable from Eq.\eqref{27} — as does q-Metropolis, whose large-repetition limit matches q-MHB \cite{25} \cite{14}. A straightforward implementation comes from modifying only the single-link update step of usual MHB\footnote{For the particular definition of \( P_q(E) \) in \cite{24}, employing escort probabilities as prescribed by TMP convention \cite{39}, one has to use slightly different definitions for q–operators. On the other hand, we employ TO convention for \( P_q(E) \) without need to escort probabilities.} in Eq.\eqref{26} to

\[
P(v_0) \rightarrow P_q(v_0) \propto \sqrt{1 - v_0^2} \exp_q (\beta N v_0) \, dv_0. \tag{33}
\]

5. Numerical results

Algorithmic performance

Whenever the equivalence of statistical ensembles holds \cite{27} reweighting methods \cite{37} allows for converting thermal averages among different ensembles. For instance Eq.\eqref{5} and Eq.\eqref{13} may be related \cite{24} by

\[
\langle O \rangle_{BG} = \left\langle \frac{O(U) e^{-S_{W}(U)}}{e^{-S_{W}(U)}} \right\rangle_{TS} / \left\langle \frac{e^{-S_{W}(U)}}{e^{-S_{W}(U)}} \right\rangle_{TS}. \tag{34}
\]

So, employing the Tsallis weight would be preferable than (and interchangeable to) the Boltzmann one when simulations become more efficient in the former ensemble.
Since statistical Monte Carlo errors are proportional to $\sqrt{2\tau_{int}}$, issues related to algorithmic efficiency may be set by computing the integrated auto-correlation time

$$
\tau_{int}(O) = \frac{1}{2} + \sum t \rho_{fO}(t).
$$

Where for a given physical observable $O$ one defines $ho_{fO} = \frac{\langle O_i O_{i+t} \rangle - \langle O_i \rangle^2}{\langle O_i^2 \rangle - \langle O_i \rangle}$. Thereby, numerical errors in Eq.(35) can be estimated by the Madras-Sokal formula [31] employing self-consistent windowing [26].

Generally a usual finite-size scaling $\tau_{int} \propto L_{side}^z$ is expected[4], and so the most efficient thermalization algorithm produces the smallest $z$-values for a set of observables. Hence correlations increase with the lattice side, one supposes that the best suited observables $O$ for performance evaluations are extended gauge-invariant quantities measured on regions of “constant physics”. This constraint may be ensured for instance by keeping the ratio $\beta = L_{side}^2/32$ fixed. In particular, we considered “critical” plaquettes of $M \times M$ size, once $M = \sqrt{2\beta \frac{1}{32}} \left(1 + \frac{1}{47}\right)$ scales with the correlation length $\xi$ of the 2d $SU(2)$ gauge theory [26].

The effects of tuning the nonextensive Tsallis parameter in the range $0.9 \leq q \leq 1.10$ were investigated while lattice volumes were set to $V = \{56^2, 64^2, 72^2, 80^2, 88^2\}$. Our $q$-generalized heat-bath algorithm and its overrelaxed version were also compared for same volumes and $q$-values. The results obtained after regression using $\tau_{int} = a \cdot L_{side}^z$, see Figure (1), indicate that simulations with $q \gtrsim 1$ are benefited by the Tsallis approach which induces considerable decrease in $\tau_{int}$. As a consequence, at largest volumes our simulations using $q = 1.1$ are up to 9% faster than the ones running under the usual (i.e. canonical) setup[7] at $q = 1.0$.

Short-time dynamic simulations

In this section we employ the previously described short-time dynamic techniques to study the finite-temperature critical behaviour of $SU(2)$ lattice gauge theory in 3d. Our simulations were started from ordered initial configurations with $m_0 = 1$, which has been proven to be an advantageous choice [43].

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[6] This $z$-exponent is not to be confused with the physical (dynamic) critical exponent $z$ measured by short-time relaxation techniques.

[7] It deserves to be noted that tuning $q$ seems to just improve the $a$ factor in $\tau_{int} = a \cdot L_{side}^z$, while the overrelaxation has a stronger impact on $z$. Thus, the typical values found for heat-bath updates imply $z \sim 1.8(1)$ without using overrelaxation, and $z \sim 1.4(1)$ (for any $q$) when this microcanonical step is added.
Figure 2: The dynamical evolution in Monte Carlo time of the Magnetization $M(t)$ [left panel] and of the cumulant $U(t)$ [right panel]. Simulations were performed for different values of $q$ in the range $[0.99,1.01]$ at the canonical critical lattice coupling $\beta = \beta_c = 3.4505$. For comparative purposes canonical (i.e. $q = 1$) simulations at $\beta = \beta_c$ (bold black line), $\beta = 0.99 \cdot \beta_c$ (bold light gray) and $\beta = 1.01 \cdot \beta_c$ (bold dark gray) are also plotted. In addition, there is a (bold dot dashed) curve at $q = 1.100$ which was tuned to the (shifted) critical coupling $\beta = (\beta_c)_T S$ in the Tsallis ensemble.

Table 1: Static and dynamic critical exponents for the 3d SU(2) pure gauge theory at its canonical critical lattice coupling $\beta \equiv \beta_c = 3.4505$, for different values of $q$ using our q-MHB algorithm, and cold starts. The data in ($q = 1.10^*$) was obtained by interpolation at the nonextensively shifted critical coupling ($\beta = 1.3275 \cdot \beta_c$). For comparisons to predictions from universality, in ($q = 1.00^*$) it is shown results for the 2d critical Ising model simulated from hot starts, and using heat-bath (HB) [33], in the BG ensemble.
Figure 3: The dynamical evolution in Monte Carlo time of the auto-correlation of the magnetization $A(t)$. The continuous bold black line is the canonical BG simulation at critical point, i.e. $q = 1$ and $\beta = \beta_c$. The other curves were simulated at fixed $q = 1.1$ and different values of lattice coupling $\beta > \beta_c$.

Figure 4: The fourth-order Binder cumulant of the Polyakov loop for $q = 1.1$ and lattice sides $L = \{64, 96, 128\}$ as a function of the lattice coupling $\beta$. The crossing happens at the critical coupling $\beta_c = \tilde{\beta}_{c,q=1.1} \approx 4.581(2)$ (in the Tsallis ensemble) where $B_4 \approx 1.825(5)$, so it is in nice agreement with predictions from universality (see text).

For each value of the Tsallis parameter, taken in the vicinity of the Boltzmannian limit $q \to 1^\pm$, we have run 5000 simulations initialized from different random seeds. The largest lattice volumes we considered $V = 128^2 \times 2$ allow for negligible finite-size effects, which was also verified by a Binder cumulant analysis in equilibrium, see below. Thus, relaxation was studied in those simulations by evolving the system during 500 steps in Monte Carlo time where the effects of nonextensivity on observables Eq.(14) and Eq.(17) was monitored. The employed statistical error analysis was standard, so data was grouped in independent blocks to compute uncorrelated standard deviations.

The results for $M(t)$ and $U(t)$ are summarized in Figure (2), which exhibits the outputs from simulations performed at $q = \{0.990, 0.999, 1.000, 1.001, 1.010\}$ at canonical critical coupling $\beta = \beta_c = 3.4505$. For comparative purposes also the data from usual canonical simulations (i.e. at Boltzmannian limit $q = 1$) with $\beta = 1.01 \cdot \beta_c$ (in bold dark gray), $\beta = \beta_c$ (in bold black) and $\beta = 0.99 \cdot \beta_c$ (in bold light gray) are shown. Moreover, there are curves of $M(t)$ and $U(t)$ (dot-dashed dark yellow) evaluated at (best approximation for) the shifted critical coupling $\beta_{TS} = 1.325 \cdot \beta_c$ for $q = 1.10$ in the Tsallis ensemble.

Under close examination, it becomes clear that our data agrees with the theoretical predictions that increasing $q$ above the unit is analogous to decrease the temperature of the system,
while the converse effect is emulated by setting $q < 1$. Thereby, the critical exponents extracted from fits of Eq. (16) and Eq. (18) are compiled in Table (1). There one finds that in a narrow range $0.999 \leq q \leq 1.001$ not only ensemble equivalence [27] but also universality arguments [30, 34] (approximately) hold when comparing data from the $SU(2)$ theory and $Z_2$ spin-system. Actually, one may suppose that an exact numerical match for such critical exponents would just happen when the shifts on the critical lattice coupling induced by nonextensive effects are properly considered.

To test that last hypothesis we have employed two different scaling methods to get “$eta_c$-shifted” (i.e., $\tilde{\beta}_{c,q}$) with $q$ fixed around the phenomenologically motivated value $q = 1.10$ [2, 11]. First, we performed a graphical matching procedure by monitoring the autocorrelation of the order parameter Eq. (19) as a function of increasing lattice couplings $\beta$, see Figure (3). Considering that an exact scaling law Eq. (20) is well-known for such observable and, $\xi_t \to \infty$ at the critical point (deconfinement transition), we could locate the nonextensively shifted critical coupling (by linear interpolation) at $\tilde{\beta}_{c,q=1.1} \approx 1.3275 \cdot \beta_c \approx 4.5805(8)$. The other approach is computationally more demanding, and complementar, once it allows for locating eventual finite-size effects quite easily [37]. It consists on evaluating, by usual simulations in equilibrium, the fourth-order Binder cumulant of the order parameter (i.e. the Polyakov Loop $W$)

$$B_4 = \frac{\langle W^4 \rangle}{\langle W^2 \rangle^2} - 3. \quad (36)$$

Then, the shifted critical coupling $\tilde{\beta}_{c,q}$ can be found at the single crossing (fixed-) point among multiple curves computed for different lattice sides. Interestingly, the value of $B_4$ at the critical point is unique for each universality class; so the $YM_{2d}$ theory is predicted [30] to have $B_4 \approx 1.832$ as the 2d Ising model [49]. In fact, our results — see Figure (4) — shows that the shifted critical coupling for $q = 1.10$ is given by $\tilde{\beta}_{c,q=1.1} \approx 4.581(2)$ where $B_4 \left( \tilde{\beta} \right) \approx 1.825(5)$, thus it also agrees with predictions from universality.

Thence, considering that $T^{-1} = a \cdot L$ and the lattice spacing $a$ is given at leading order by $a \sim 1/\beta \cdot \sqrt{x}$ [50], we may conclude that the deconfinement critical temperature is really shifted upwards up to 30% by nonextensive effects when $q = 1.10$, as it was previously hypothesized.

In this same vein, we see from compiled data in Table (1) that critical exponents $z = 2.139(9)$ and $\beta/\nu = 0.124(4)$ of the $YM_{2d}$ gauge theory simulated at $q = 1.10$ — with the corrected critical coupling $\tilde{\beta}_{c,q=1.1} \approx 4.5805(8)$ — are compatible with computations in the BG ensemble (i.e., using $q = 1.0$ and $\beta_c = 3.4505$), to know $z = 2.008(8)$ and $\beta/\nu = 0.127(5)$. Besides that, the results nicely agree with values from literature for the critical 2d Ising model in the BG ensemble [33], where $z = 2.155(3)$ and $\beta/\nu = 0.125$. These are nontrivial evidences that the universality hypothesis among such systems [30] holds even when they are studied in different (but equivalent, see [27]) ensembles.

6. Concluding remarks

We have designed a generalized hybrid heat-bath algorithm ($q$-MHB) to perform ab initio simulations of $SU(2)$ lattice gauge fields on the nonextensive ensemble of Tsallis. The algorithm emerges as an exact solution for a generalized detailed balance equation already proposed in [25]. Through group embedding this scheme can be adapted to any gauge group $SU(N)$. Then, to verify the numerical performance of the algorithm, as a function of $q$, we checked the scaling $\tau_{int} = a \cdot L^{z_{side}}$ of the integrated correlation time of an extended critical plaquette. We have observed that employing the generalized ensemble of Tsallis with $q > 1$ in association to overrelaxation allowed for improvements on simulation performance of up to 9%.

As discussed by Morishita [27] the Tsallis parameter $q$ may be physically interpreted as the strenght of an effective thermal coupling to a finite heat-bath. More explicitly, by considering the heat capacity of that bath to be $C_v^{HB}$ and $k$ as a constant with proper dimension, one has $q = 1 - \frac{k}{C_v^{HB}}$. Then, the canonical Boltzmann-Gibbs ensemble is recovered when $C_v^{HB} \to \infty$,
which implies the $q \to 1^-$ limit. On the other hand, in the oposite regime, the microcanonical ensemble of Boltzmann emerges when $C_{v}^{HB} \to 0^+$, i.e. when $q < 0$. Both such limits obey $C_{v}^{HB} \geq 0$ and so are said to be weakly coupled.

The remaining mathematical possibility is to chose $C_{v}^{HB} < 0$ to produce $q > 1$. This elusive regime is known as strongly coupled, in the sense that its thermal fluctuations are stronger than in the canonical/microcanonical limits. From a purely computational viewpoint it has been proved that simulations with $q > 1$ are equivalent to ones in the multicanonical ensemble (MUCA) of Berg [51]. Thus, while the strongly coupled nonextensive approach is the most efficient one in reducing tunneling-times around phase transitions, as also corroborated by our performance analysis, the physical interpretation of negative heat capacities of reservoirs is still debated.

Furthermore, we have employed our generalized heat-bath algorithm to study the short-time (relaxation) dynamics of the SU(2) gauge theory in the Tsallis ensemble [47]. To do so, a serie of (initially orderly) gauge configurations was prepared and then evolved during some hundred Monte Carlo steps. During such a temporal evolution a set of observables Eq.(14), Eq.(17) and Eq.(19) was measured. After that, power-law scaling relations Eq.(16), Eq.(18) and Eq.(20) were carefully adjusted to data to obtain the (static and dynamic) critical exponents collected on Table (1). By considering only the regions with best fit-qualities ($\chi^2$/dof $\simeq 1$) we have verified that long-standing universality arguments of [30] hold for the 2d Ising model, in BG ensemble, and the critical SU(2) gauge theory at Tsallis ensemble. Notwithstanding, to ensure such a perfect matching, the nonextensively induced shift on the lattice coupling ($\beta_c \to \tilde{\beta}_{c,q\neq1}$) had to be precisely calculated.

To determine that shift of the critical gauge coupling as a function of $q$ we have proposed a new approach based on finite-size scaling. Here a nonequilibrium scaling relation Eq.(20) was fitted to data while varying $\beta$ to locate the new critical region in the Tsallis ensemble (i.e., whenever $q \neq 1$). The method so introduced was successfully compared with a traditional one, the fourth-order Binder cumulant. In addition, both approaches agree that deconfinement temperature is increased by about 30% when a phenomenologically favoured value $q = 1.10$ was employed [2, 11].

Once nonextensive simulation setups analogous to ones here presented are applicable to lattice QCD, one would expect to be able to describe early nonequilibrium stages of hadronic collisions from first principles. For instance, it would be interesting to cross-check how universal nonextensive effects relate the 3d O(4) model — accessible through algorithms on section IV, and [27] — and QCD. Finally, further pieces of encouragement in this direction is that the Tsallis framework is well suited to describe systems showing power-law relaxation in time and energy, as well as those relaxing by nonergodic occupation of phase space due to unusual underlying microscopic dynamics. All these peculiar features are typically found during transient times of hadronic collisions [11, 12, 16, 48].

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