

Equation of state of Yang-Mills theories: results and new methods on the lattice

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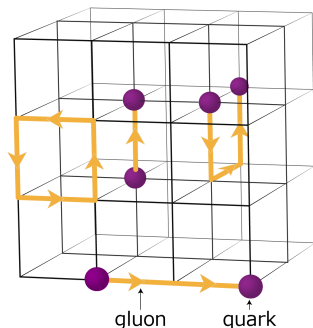
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In QFTs, the **regularization on the lattice** is an incredibly powerful tool for the calculation of a very large and varied set of physical observables, especially in **QCD** and **QCD-like** theories.

It provides *the* mathematically well-defined **non-perturbative** formulation of QCD, defined for *any* value of the coupling.

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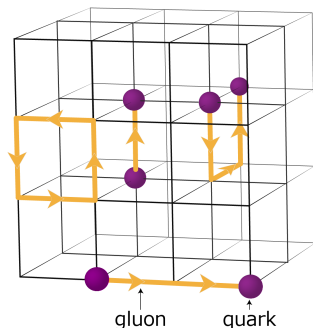


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The action

For $SU(N)$ Yang-Mills theories regularized on the lattice, the dynamics can be described by the **Wilson action**

$$S_W = -\frac{\beta}{N} \sum_x \sum_{0 \leq \mu < \nu \leq 3} \text{Tr} U_{\mu\nu}(x)$$

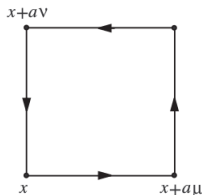
where $U_{\mu\nu}$ is the **plaquette** and β the inverse coupling $\frac{2N}{g^2}$.

The expectation value of an observable \mathcal{O} is

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \prod_{n,\mu} dU_\mu \mathcal{O}(U_\mu) e^{-S_W}$$

and can be computed via **Monte Carlo integration**. Z is the partition function

$$Z = \int \prod_{x,\mu} dU_\mu(x) e^{-S_W}$$



Equation of state of Yang-Mills theories

- One of the main features of $SU(N)$ Yang-Mills gauge theories is the existence of a **deconfinement phase transition**, i.e. a temperature above which gluons are “deconfined”.
- In general, thermal properties of QCD and QCD-like theories are particularly well suited for being studied on the lattice, due to **non-perturbative** nature of the deconfinement transition.
- The low-temperature phase ($T < T_c$) can be studied with great accuracy and lattice results close to the critical temperature can be compared with a gas of massive, non-interacting hadrons (\rightarrow **HRG model**).
- For Yang-Mills theories this is even more dramatic: our goal is to compare lattice data for $SU(2)$ and $SU(3)$ in the confining region with the prediction of a glueball gas with an Hagedorn spectrum.

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- this study focuses on the **pure gauge** sector of the theory (it retains most of the non trivial features of the full theory + Monte Carlo computations are faster and more precise + technical difficulties of fermion regularization are avoided)
- in the confining phase the **only** degrees of freedom are **glueballs**: looking at the thermodynamics in the confining phase we have a tool to **investigate the glueball spectrum of the theory**
- our main result is that the thermodynamics of the model can only be described assuming a **Hagedorn** spectrum, i.e. a **string-like** description of glueballs → highly non trivial test of the effective string picture of confinement
- this work is meant as a continuation of previous studies for the $SU(3)$ YM theory [Meyer, 2009; Borsányi et al., 2012] and for $SU(N)$ theories in 2+1 dimensions [Caselle et al., 2011]
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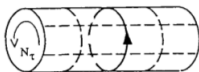
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- the theory at nonzero temperature is defined on an asymmetric hypercubic lattice of size $a^4(N_t \times N_s^3)$, where a is the lattice spacing
- the temperature is determined by the inverse of the temporal extent (with periodic boundary conditions): $T = (aN_t)^{-1}$



The thermodynamic quantities taken into account will be:

- the **pressure** $p \simeq \frac{T}{V} \log Z(T, V)$ (for $V \rightarrow \infty$)
- the **trace of the energy-momentum tensor** $\Delta = \epsilon - 3p$
- the energy density $\epsilon = \Delta + 3p$
- the entropy density $s = \frac{\epsilon+p}{T} = \frac{\Delta+4p}{T}$

On the lattice, the **pressure** can be estimated by the means of the so-called “integral method” [Engels et al., 1990]:

$$\frac{p}{T^4} = -6N_t^4 \int_0^\beta d\beta' (U_T - U_0)$$

where U_T and U_0 are **plaquette expectation values** at T and zero temperature.

The **trace of energy-momentum tensor** (also called **trace anomaly**) is simply

$$\frac{\Delta}{T^4} = \frac{\epsilon - 3p}{T^4} = T \frac{\partial}{\partial T} \left(\frac{p}{T^4} \right) = -6N_t^4 T \frac{\partial \beta}{\partial T} (U_T - U_0).$$

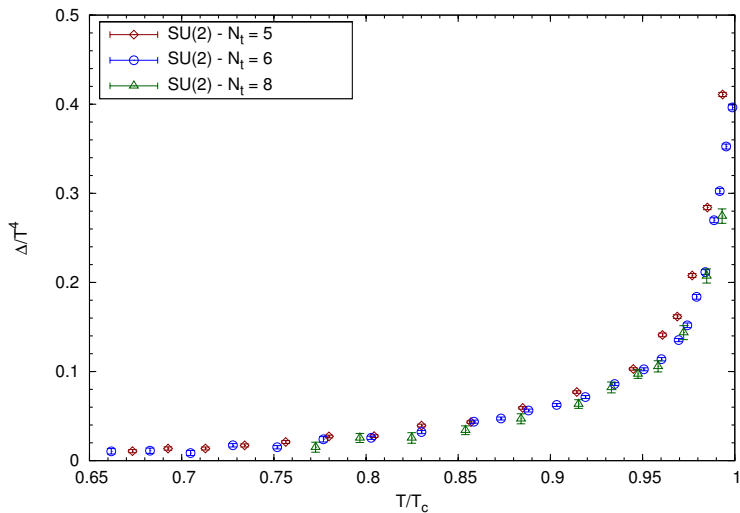
The SU(2) model is a perfect laboratory to test these results:

- the deconfinement transition is of second order (this fixes the Hagedorn temperature $T_H \equiv T_c$)
- the infrared physics of the model is very similar to that of the SU(3) theory, with one important difference: for SU(2) only $C = 1$ glueballs exist. The comparison with SU(3) should be very insightful!

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SU(2): trace of energy-momentum tensor



The behaviour of the system is supposed to be dominated by a **gas of non-interacting glueballs**.

The prediction of an ideal relativistic Bose gas can be used to describe the thermodynamics of such gas. The pressure is

$$p = \frac{T}{V} \log Z = 2(2J + 1) \left(\frac{m^2}{2\pi} \right)^2 \sum_{k=1}^{\infty} \left(\frac{T}{km} \right)^2 K_2 \left(k \frac{m}{T} \right)$$

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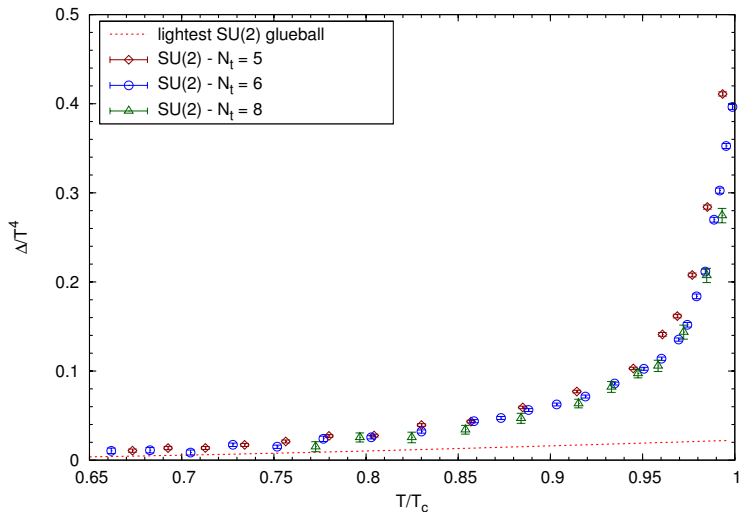
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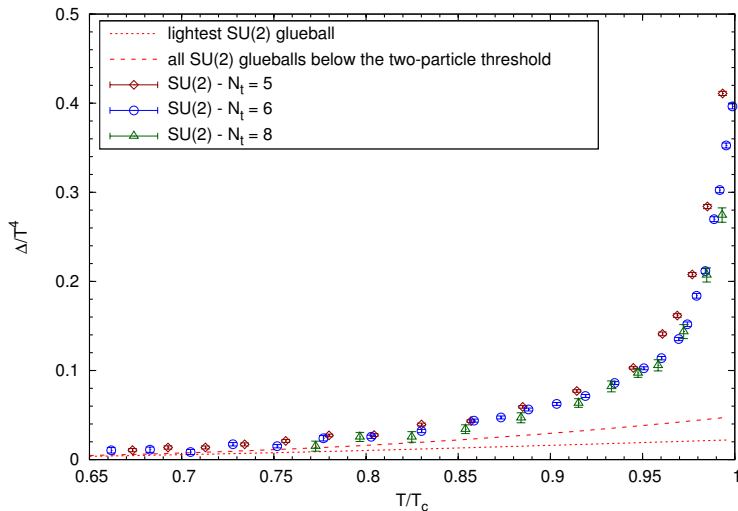
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SU(2): trace of energy-momentum tensor



Contribution of the lowest glueball state 0^{++} compared with the data

SU(2): trace of energy-momentum tensor



Contribution of all SU(2) glueball states with mass $m < 2m_{0^{++}}$

- Usually the thermodynamics of the system is saturated by the first state (or, in some cases, the few lowest states) of the spectrum due to the exponential dependence on the mass.
- The large gap between the $m_{0^{++}}$ and the $m < 2m_{0^{++}}$ curves and those between them and the data show that the spectrum must be of the **Hagedorn** type, i.e. that the number of states increases exponentially with the mass.
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Closed string models for the glueball spectrum exist since the '80s [Isgur&Paton, 1985]

In this approach glueballs are described in the limit of large masses as **“rings of glue”**, that is **closed tubes of flux modelled by closed bosonic string states**

A simple but precise prediction is that these states must have an exponential spectral density:

$$\hat{\rho}(m) = \frac{(D-2)^{D-1}}{m} \left(\frac{\pi T_H}{3m} \right)^{D-1} e^{m/T_H}$$

where the **Hagedorn temperature** [Hagedorn, 1965] is defined as

$$T_H = \sqrt{\frac{3\sigma}{\pi(D-2)}}$$

This result can be used in combination with the glueball gas to account for the contribution of the states above the mass threshold $2m_{0++}$:

$$\Delta = \sum_{m < 2m_{0++}} (2J+1)\Delta(m, T) + \int_{2m_{0++}}^{\infty} dm \hat{\rho}(m) \Delta(m, T)$$

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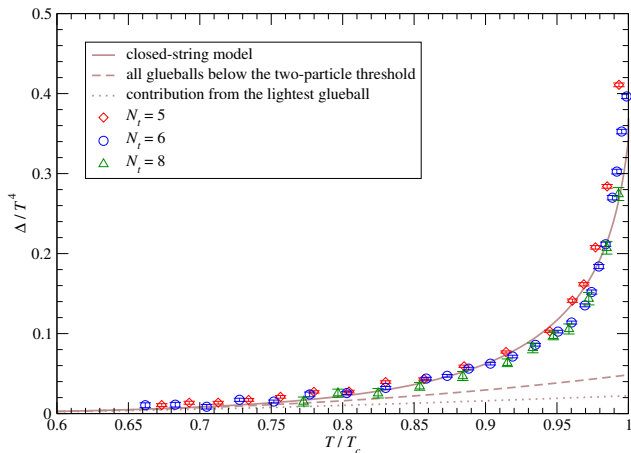
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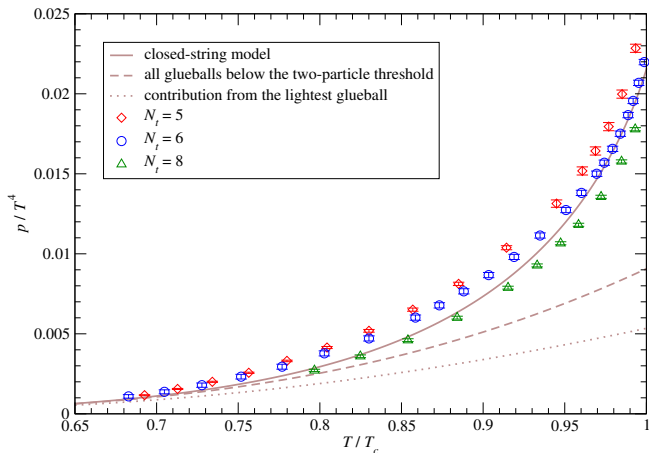
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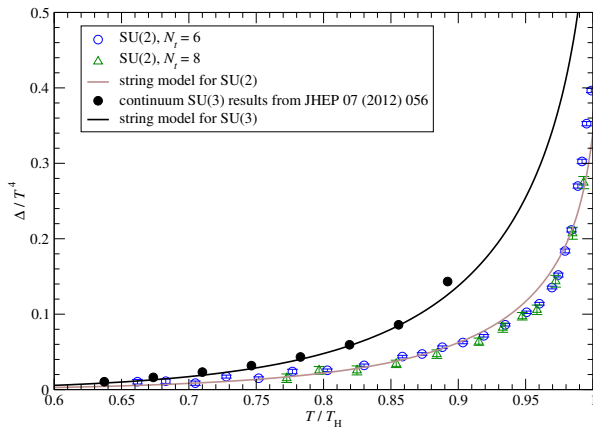
For $N = 2$ we have that $T_H = T_c$, as the deconfinement transition is 2nd order



- SU(3) has **complex** representations, thus glueballs have both $C = +1/ - 1$ and the spectrum contains **approximately twice** the number of glueballs with respect to SU(2)
- SU(3) has a **first order** deconfinement transition, so $T_c < T_H$: we can fix T_H at the expected Nambu-Goto value:

$$T_H = \sqrt{\frac{3\sigma}{2\pi}} \simeq 0.691\sqrt{\sigma} = 1.098 T_c$$

where $\sqrt{\sigma} \simeq 440$ MeV is the string tension



The doubling of the Hagedorn spectrum is clearly visible in the data!

Alternative approach:

- take into account effects due to the finite size (and thus of repulsive interactions) of glueballs using a modified chemical potential in the glueball gas

$$\mu_j^* = b_j \mu_B + q_j \mu_Q + s_j \mu_S - v_j p$$

- the eigenvolume of each species is $v_j = \frac{16\pi}{3} r_j^3 \rightarrow$ “effective” radius
- already used for QCD in the HRG

Three possible ansätze for the radii of the glueball states have been considered:

- r directly proportional to $m^{1/3}$
- r inversely proportional to $m^{1/3}$
- fixed radius

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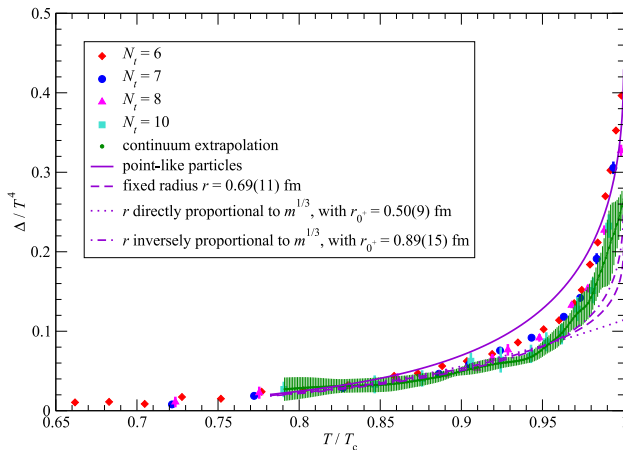
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Excluded Volume effects in SU(2)



The best result is obtained with the volume inversely proportional to the mass, both for SU(2) and SU(3) \rightarrow both fits yield similar radii for the 0^{++}

- thermodynamics of $SU(2)$ and $SU(3)$ Yang-Mills theories in $D = (3 + 1)$ are well described by a gas of **non-interacting** glueballs
- good agreement¹ is obtained only assuming a **Hagedorn spectrum** for the glueballs, whose fine details agree well with the **effective string** prediction
- a slightly alternative approach yields excellent results including **excluded volume** effects²

¹M. Caselle, A. N. and M. Panero, JHEP **07** (2015) 143, [arXiv:1505.01106]

²P. Alba, W. Alberico, A. N., M. Panero and H. Stöcker, under peer review process, [arXiv:1611.05872]

Applications of Jarzynski's relation in lattice gauge theories

In lattice gauge theories the expectation values of a large set of physical quantities is *naturally* related to the computation (via Monte Carlo simulations) of free-energy differences.

For example:

- equilibrium thermodynamics (pressure)
- 't Hooft loops
- magnetic susceptibility of strongly interacting matter

In many cases the calculation of ΔF is a **computationally challenging** problem: this motivates the search for new methods and algorithms.

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Jarzynski's equality [Jarzynski, 1997] relates the **exponential statistical average of the work** done on a system during a non-equilibrium process with the difference between the initial and the final **free energy** of the system.

For an isothermal transformation it can be written as

$$\left\langle \exp \left(-\frac{W(\lambda_i, \lambda_f)}{T} \right) \right\rangle = \exp \left(-\frac{\Delta F}{T} \right)$$

The evolution of the system is performed by changing (continuously or discretely) a chosen set λ of one or more parameters, such as the couplings or the temperature of the system.

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- on the r.h.s. $\exp \left(-\frac{\Delta F}{T} \right) = \frac{Z(T, \lambda_f)}{Z(T, \lambda_i)}$ where $\Delta F = F(\lambda_f) - F(\lambda_i)$
- $W(\lambda_i, \lambda_f)$ is the **work** made on the system to change the control parameter from λ_i to λ_f . If the transformation is discrete (like a Markov chain in MC simulations), then the process is divided into N steps and the total work is

$$W(\lambda_i \equiv \lambda_0, \lambda_f \equiv \lambda_N) = \sum_{n=0}^{N-1} (H_{\lambda_{n+1}}[\phi_n] - H_{\lambda_n}[\phi_n])$$

where ϕ_n is the configuration of the variables of the system at the n -th step of the transformation

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- on the r.h.s. $\exp \left(-\frac{\Delta F}{T} \right) = \frac{Z(T, \lambda_f)}{Z(T, \lambda_i)}$ where $\Delta F = F(\lambda_f) - F(\lambda_i)$
- $W(\lambda_i, \lambda_f)$ is the **work** made on the system to change the control parameter from λ_i to λ_f . If the transformation is discrete (like a Markov chain in MC simulations), then the process is divided into N steps and the total work is

$$W(\lambda_i \equiv \lambda_0, \lambda_f \equiv \lambda_N) = \sum_{n=0}^{N-1} (H_{\lambda_{n+1}}[\phi_n] - H_{\lambda_n}[\phi_n])$$

where ϕ_n is the configuration of the variables of the system at the n -th step of the transformation

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- The equality requires no particular assumptions and holds under very general conditions (e.g. the detailed balance condition for Markov chains)
- It can be extended for non-isothermal transformations [Chatelain, 2007]
- In Monte Carlo simulations we can control
 - N , the number of steps for each transformation between initial and final value of the parameter λ
 - n_r , the number of "trials", i.e. realizations of the non-equilibrium transformation
- A systematic **discrepancy** appears between the results of the 'direct' ($\lambda_i \rightarrow \lambda_f$) and the 'reverse' ($\lambda_f \rightarrow \lambda_i$) transformation. One has to choose a suitable combination of N and n_r in order to obtain convergence.

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Interfaces in the \mathbb{Z}_2 gauge model

The \mathbb{Z}_2 gauge model in 3 dimensions is the simplest lattice gauge theory in which to study interfaces \rightarrow Wilson action with \mathbb{Z}_2 variables; **confining** phase for small values of the inverse coupling β_g . It can be exactly rewritten as the 3-dimensional Ising model on the **dual** lattice:

$$H = -\beta \sum_{x,\mu} J_{x,\mu} \sigma_x \sigma_{x+a\hat{\mu}} \quad \text{with } \beta = -\frac{1}{2} \ln \tanh \beta_g$$

To create an interface we induce a **frustration** on the system, by imposing $J_{x,\mu} = -1$ only for the couplings in a specific slice of the lattice (and only in one direction) and setting the remaining ones to 1.

The **free energy** associated with this interface is

$$\frac{Z_a}{Z_p} = N_0 \exp(-F^{(1)})$$

- Z_p : **periodic** boundary conditions (all couplings set to $J_{x,\mu} = 1$)
- Z_a : **antiperiodic** boundary conditions (couplings between two slices are set to $J_{x,\mu} = -1$)

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Results in the \mathbb{Z}_2 gauge model

We can compute the Z_a/Z_p ratio with Jarzynski's relation by gradually varying the couplings $J_{x,\mu}$ from 1 to -1 (and viceversa):

$$J_{x,\mu}(n) = 1 - \frac{2n}{N}$$

where N is the total number of steps between periodic ($J_{x,\mu}(0) = 1$) and antiperiodic ($J_{x,\mu}(N) = -1$) boundary conditions.

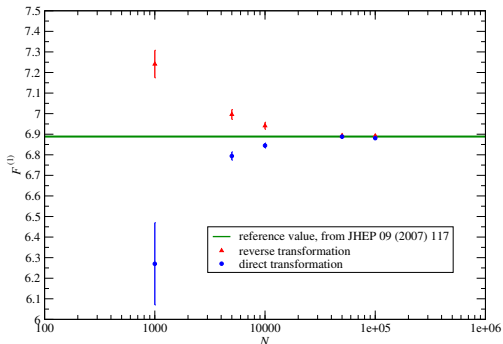
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$$\beta = 0.223102, \quad N_0 = 96, \quad N_1 = 24, \quad N_2 = 64$$



The results from 'direct' and 'reverse' transformations converge to older results when N is large enough.

The results obtained changing the interface size L can be compared with the analytical prediction of the **effective string model**.

Benchmark study: pressure in $SU(N)$ gauge theories

The **pressure** p in the thermodynamic limit equals the opposite of the free energy density

$$p \simeq -f = \frac{T}{V} \log Z(T, V)$$

and a common way to estimate it on the lattice is using the so-called “integral method” [Engels et al. (1990)]:

$$p(T) = \frac{1}{a^4} \frac{1}{N_t N_s^3} \int_0^{\beta_g(T)} d\beta'_g \frac{\partial \log Z}{\partial \beta'_g}$$

where the integrand is calculated from plaquette expectation values.

Jarzynski's relation gives us a direct method to compute the pressure: we can change the parameter β_g controlling the temperature T in a non-equilibrium transformation!

The **difference of pressure** between two temperatures T and T_0 is

$$\frac{p(T)}{T^4} - \frac{p(T_0)}{T_0^4} = \left(\frac{N_t}{N_s}\right)^3 \ln \langle e^{-W_{\text{SU}(N_c)}} \rangle$$

with $W_{\text{SU}(N_c)}$ being the "work" made on the system:

$$W_{\text{SU}(N_c)} = \sum_{n=0}^{N-1} \left[S_W(\beta_g^{(n+1)}, \hat{U}) - S_W(\beta_g^{(n)}, \hat{U}) \right];$$

here S_W is the standard Wilson action and \hat{U} is a configuration of $\text{SU}(N_c)$ variables on the links of the lattice.

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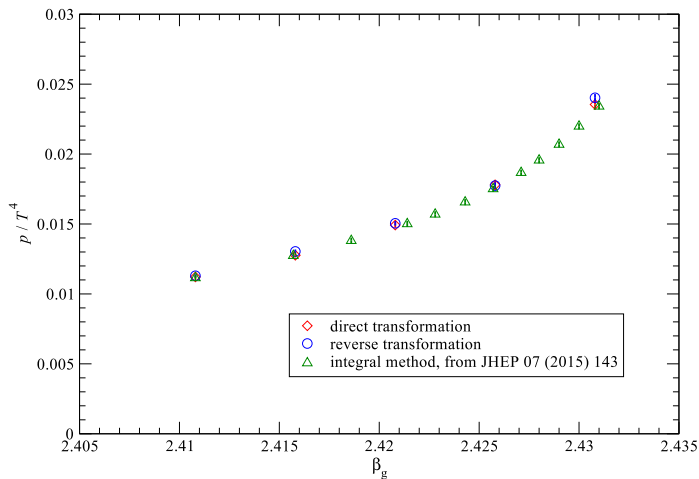
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Preliminary results for the SU(2) model



Excellent agreement with integral method data [Caselle et al., 2015] but using a fraction of CPU time.

Jarzynski's equality allows for new ways of computing free-energy differences in lattice gauge theories. A method based on this relation has been tested¹ for the computation of two different physical quantities:

- the free energy of an interface in the \mathbb{Z}_2 gauge model
- the pressure in the confining region of the $SU(2)$ gauge model

In both cases the method proved to be perfectly reliable with a suitable choice of N and n_r ; moreover the computational efficiency is comparable and in many cases superior to standard methods.

¹M. Caselle, G. Costagliola, A. N., M. Panero and A. Toniato, Phys. Rev. **D94** (2016), no. 3 034503, [arXiv:1604.05544]

- In principle there are no obstructions to the derivation of numerical methods based on Jarzynski's relation for **fermionic** algorithms, opening the possibility for many potential applications in full QCD
- One example is the calculation of the free energy density in QCD with a **background magnetic field** B , in order to measure the magnetic susceptibility of the strongly-interacting matter.

Methods based on Jarzynski's relation can be applied in order to perform non-equilibrium transformations in which the field B itself is changed gradually.

- Another interesting application that we envision is in studies involving the **Schrödinger functional**: Jarzynski's relation could be used to compute changes in the transition amplitude $Z_{\mathcal{I},\mathcal{F};L}$ induced by a change in the parameters that specify the initial (\mathcal{I}) and final (\mathcal{F}) states on the boundaries.

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Thanks for your attention!

The SU(2) scale setting is fixed by calculating the string tension via the computation of **Polyakov loop correlators** with the multilevel algorithm. The interquark potential is extracted using

$$V = -\frac{1}{N_t} \log \langle PP \rangle$$

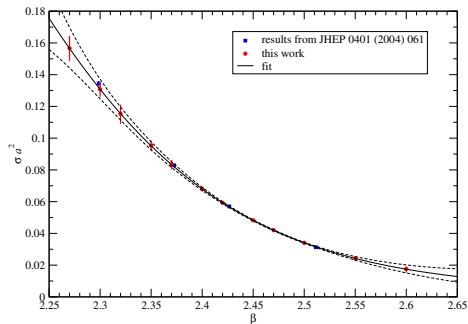
and the string tension is calculated by fitting V for different values of r using

$$V = \sigma r + V_0 - \frac{\pi}{12r}.$$

The values of the string tension are interpolated by a fit to

$$\log(\sigma a^2) = \sum_{j=0}^{n_{\text{par}}-1} a_j (\beta - \beta_0)^j \quad \text{with } \beta_0 = 2.40 \text{ and } n_{\text{par}} = 4$$

Results are presented below along with older data¹.

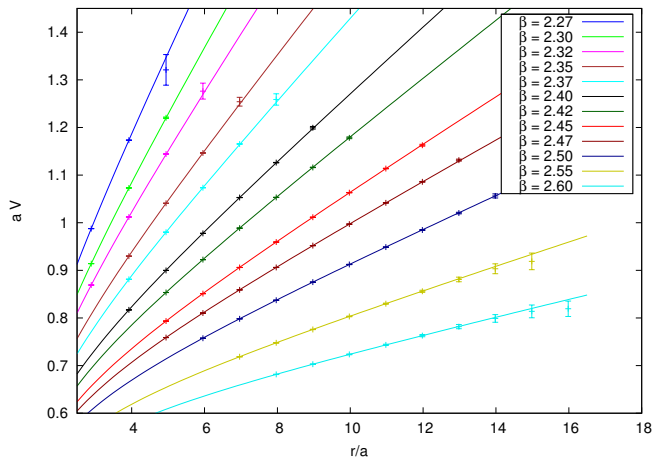


¹B. Lucini, M. Teper, U. Wenger, *The high temperature phase transition in SU(N) gauge theories*, 2003

β	r_{\min}/a	σa^2	aV_0	χ_{red}^2
2.27	2.889	0.157(8)	0.626(14)	0.6
2.30	2.889	0.131(4)	0.627(30)	0.1
2.32	3.922	0.115(6)	0.627(32)	2.3
2.35	3.922	0.095(3)	0.623(20)	0.2
2.37	3.922	0.083(3)	0.621(18)	1.0
2.40	4.942	0.068(1)	0.617(10)	1.4
2.42	4.942	0.0593(4)	0.613(5)	0.1
2.45	4.942	0.0482(2)	0.608(4)	0.4
2.47	4.942	0.0420(4)	0.604(5)	0.3
2.50	5.954	0.0341(2)	0.599(2)	0.1
2.55	6.963	0.0243(13)	0.587(11)	0.2
2.60	7.967	0.0175(16)	0.575(16)	0.3

Table : *

Results for the string tension in units of the inverse squared lattice spacing at different values of the Wilson action parameter β (first column). V was extracted from Polyakov loop correlators on lattices of temporal extent $L_t = 32a$.



N_s^4 at $T = 0$	$N_s^3 \times N_t$ at $T \neq 0$	n_β	β -range	n_{conf}
32^4	$60^3 \times 5$	17	[2.25, 2.3725]	1.5×10^5
40^4	$72^3 \times 6$	25	[2.3059, 2.431]	1.5×10^5
40^4	$72^3 \times 8$	12	[2.439, 2.5124]	10^5

Table : *

The first two columns show the lattice sizes (in units of the lattice spacing a) for the $T = 0$ and finite-temperature simulations, respectively. In the third column, n_β denotes the number of β -values simulated within the β -range indicated in the fourth column. Finally, in the fifth column we report the cardinality n_{conf} of the configuration set for the $T = 0$ and finite- T simulations.

The **mass spectrum** of a closed strings gas in D spacetime dimensions is given by

$$m^2 = 4\pi\sigma \left(n_L + n_R - \frac{D-2}{12} \right)$$

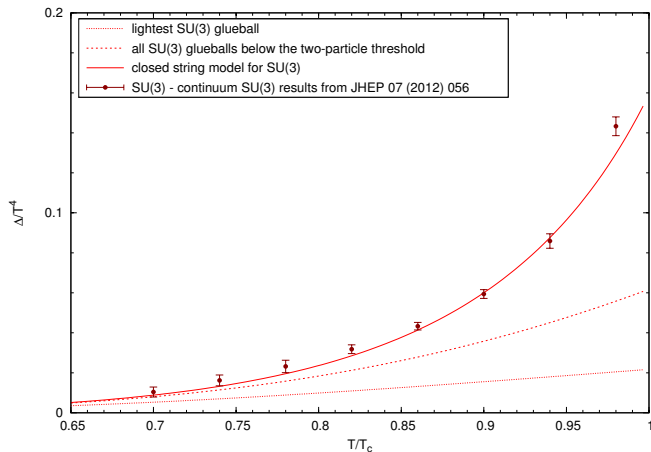
where $n_L = n_R = n$ are the total contribution of left- and right-moving phonons on the string.

Every glueball state corresponds to a given phonon configuration, but associated to each fixed n there are multiple different states whose number is given by $\pi(n)$, i.e. the **partitions** of n .

The **density of states** $\rho(n)$ is expressed through the square of $\pi(n)$

$$\rho(n) = \pi(n_L)\pi(n_R) = \pi(n)^2 \simeq 12(D-2)^{\frac{D-1}{2}} \left(\frac{1}{24n} \right)^{\frac{D+1}{2}} \exp \left(2\pi \sqrt{\frac{2(D-2)n}{3}} \right).$$

SU(3): trace of energy-momentum tensor



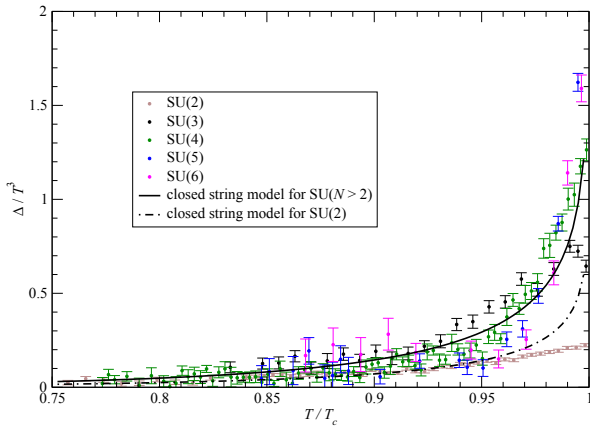
Also in this case the $m < 2m_{0^{++}}$ sector of the glueball spectrum is not enough to fit the behaviour of Δ/T^4 , while including the whole Hagedorn spectrum we find again a remarkable agreement (with no free parameter!)

The same picture is confirmed by a study performed a few years ago¹ in (2+1) dimensional SU(N) Yang-Mills theories for $N = 2, 3, 4, 6$. Also in this case:

- a Hagedorn spectrum was mandatory to fit the thermodynamic data
- there was a jump between the SU(2) and the SU($N > 2$) case due to the doubling of the spectrum
- we had to fix the Hagedorn temperature to the Nambu-Goto value which, due to the different number of transverse degrees of freedom is different from the (3+1) dimensional one: $T_H = \sqrt{3\sigma/\pi} \simeq 0.977\sqrt{\sigma}$

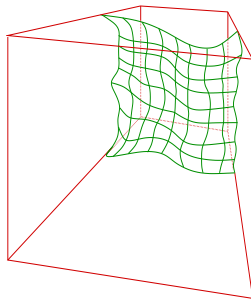
¹M. Caselle et al., *Thermodynamics of SU(N) Yang-Mills theories in 2+1 dimensions I - The confining phase*, 2011

SU(N) Yang-Mills theories in (2 + 1) dimensions



Why study interfaces?

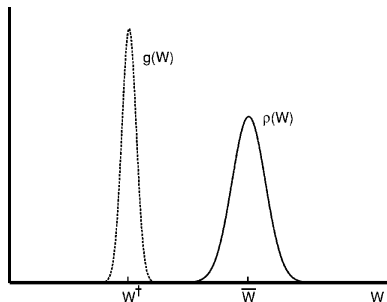
- experimental applications in condensed matter systems
- appear in many contexts also in HEP (“domain walls” at finite T , 't Hooft loops)
- also related to flux tubes in confining gauge theories which can be studied with string-theory tools



With this method (using $N \simeq 10^6$ steps and $n_r \simeq 10^3$ trials) we obtained high-precision results at fixed β and for different interface size L .

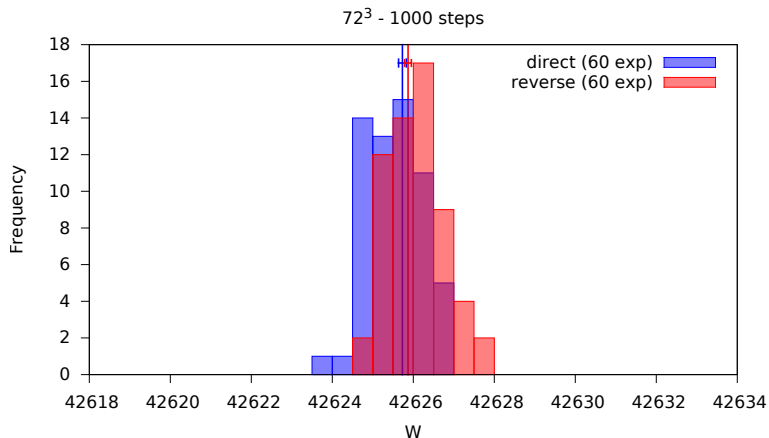
These results can be compared with the analytical prediction of the [effective string model](#) which describes the transverse fluctuations of the interface at low energy.

In particular, choosing the [Nambu-Goto](#) action as S_{eff} , one can look at the [difference](#) between numerical results and the NG prediction and examine its dependence on the size L of the interface, in order to understand the nature of the terms that do not arise from the NG low-energy expansion.

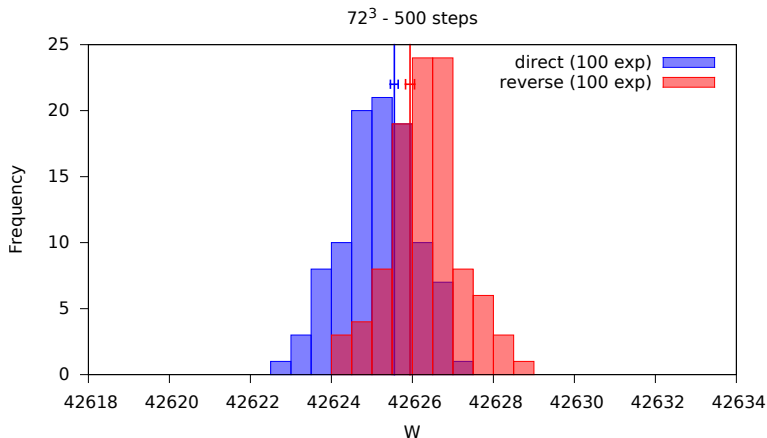


Picture taken from [Jarzynski (2006)]

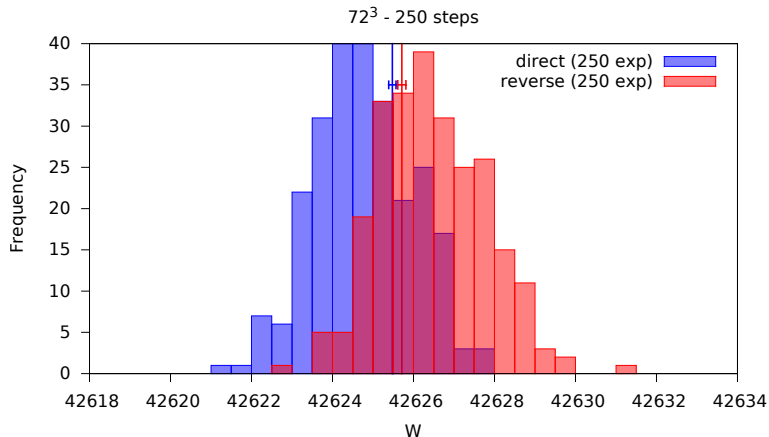
In most realizations the work is statistically distributed on $\rho(W)$; however the trials that dominate the exponential average are in the region where $g(W) = \rho(W)e^{-\beta W}$ has the peak.



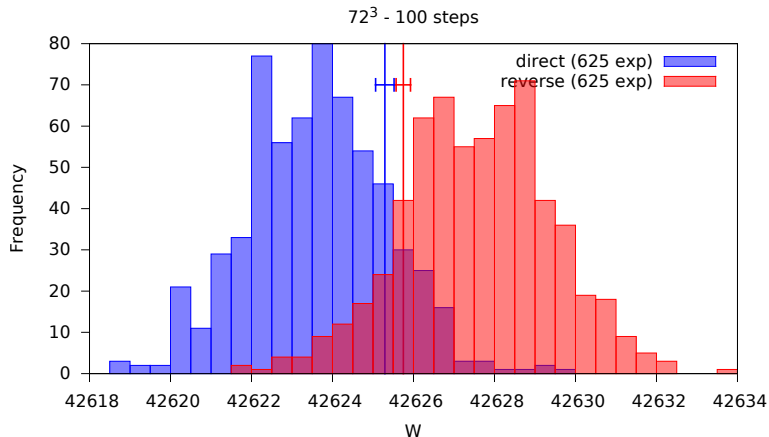
Values of total work W for different transformations $\beta = 2.4158 \leftrightarrow 2.4208$ for $N_t = 6$ in SU(2) theory. Vertical lines indicate the value of the free energy difference ΔF obtained from these trials (with the corresponding error).



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Eliminating the vacuum contribution

The pressure is normalized to the value of $p(T)$ at $T = 0$ in order to remove the contribution of the vacuum. Using the 'integral method' the pressure can be rewritten (relative to its $T = 0$ vacuum contribution) as

$$\frac{p(T)}{T^4} = -N_t^4 \int_0^\beta d\beta' [3(P_\sigma + P_\tau) - 6P_0]$$

where P_σ and P_τ are the expectation values of spacelike and timelike plaquettes respectively and P_0 is the expectation value at zero T .

Using Jarzynski's relation one has to perform another transformation $\beta_i \rightarrow \beta_f$ but on a symmetric lattice, i.e. with lattice size \tilde{N}_s^4 instead of $N_t \times N_s^3$. The finite temperature result is then normalized by removing the $T = 0$ contribution calculated this way.

$$\frac{p(T)}{T^4} = \frac{p(T_0)}{T_0^4} + \left(\frac{N_t}{N_s}\right)^3 \ln \frac{\left\langle \exp \left[-W_{\text{SU}(N_c)}(\beta_g^{(0)}, \beta_g)_{N_t \times N_s^3} \right] \right\rangle}{\left\langle \exp \left[-W_{\text{SU}(N_c)}(\beta_g^{(0)}, \beta_g)_{\tilde{N}^4} \right] \right\rangle^\gamma}$$

with $\gamma = (N_s^3 \times N_0) / \tilde{N}^4$.

$$\left\langle \exp \left(- \sum_{n=0}^{N-1} \left\{ \frac{H_{\lambda_{n+1}}[\phi_n]}{T_{n+1}} - \frac{H_{\lambda_n}[\phi_n]}{T_n} \right\} \right) \right\rangle = \frac{Z(\lambda_N, T_N)}{Z(\lambda_0, T_0)}$$