Thermodynamics of strongly-coupled lattice QCD in the chiral limit

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Let us consider $U(N_c)$ lattice QCD, with $N_f = 1$ massless staggered fermion, on a $N_s^3 \times N_t$ lattice, at finite temperature.

- The Goldstone boson, associated with the spontaneous breaking of the remnant $U(1)$ chiral symmetry, is interacting ($f_\pi^2 \neq 0$). But, in the $T \ll f_\pi$ regime, it is essentially a free particle. At low temperatures, it is expected to behave like a Stefan-Boltzmann gas.

- We study the thermal properties of $U(3)$ and $SU(3)$ lattice QCD, in the strong lattice coupling limit ($\beta = 0$) and chiral limit ($m_q = 0$), with a focus on the expected (near) ideal gas behavior.

- Possibility of using algorithms (of the worm type), which are very efficient in strong and chiral limits, and at low temperatures.

- Precursor to an extensive precision study of the equation of state of lattice QCD, in the strong coupling limit: finite quark mass, baryon density, etc.
Thermodynamics of a free massless boson on the lattice

The thermal properties of free massless bosons on a $N_s^3 \times N_t$ anisotropic lattice, with anisotropy $\gamma = \frac{a}{a_t}$, have been studied in detail. [Karsch-Engels-Satz '82]

**Energy density:**

\[
a^4(\varepsilon - \varepsilon_0) = -\frac{\gamma^3}{N_s^3 N_t} \sum_{\vec{j} \neq 0} \frac{\sin^2 (\pi j_0 / N_t)}{b^2 + \gamma^2 \sin^2 (\pi j_0 / N_t)}, \quad b^2 = \sum_{i=1}^{3} \sin^2 (\pi j_i / N_s)
\]

\[
a^4 \varepsilon_0 = \frac{\gamma^3}{N_s^3} \sum_{\vec{j}} \left( b^2 + \gamma^2 + b\sqrt{\gamma^2 + b^2} \right)^{-1}
\]

**Interaction energy:**

(holds on any finite lattice)

\[
\varepsilon - 3p = 0
\]

**Lessons:**

- Finite-size effects are considerable
- For mild lattice corrections, use: $N_s \geq 2N_t$ and $\gamma \geq 2$
- Ideal gas behavior in the $\gamma \to \infty$ (continuous time) limit
Analytical integration over $U_{x\mu}$ and $\psi_x, \bar{\psi}_x$ in $U(3)$ lattice QCD yields the partition function of a **monomer-dimer system**: [Rossi-Wolff '84]

\[
Z = \int DU D\psi D\bar{\psi} e^{2a_t m_q \sum_x \bar{\psi}_x \psi_x + \sum_{x,\mu} \gamma^{\delta_{\mu 0}} \eta_{x\mu} (\bar{\psi}_x U_{x\mu} \psi_x + \hat{\mu} - h.c.)}
\]

\[
= \sum_{\{n,k\}} \left( \prod_{x,\mu} \frac{(3 - k_{x\mu})!}{3! k_{x\mu}!} \right) (2a_t m_q)^{N_M} \gamma^{2 N_{Dt}}
\]

$n_x, k_{x\mu} \in \{0, 1, 2, 3\}$, \hspace{1cm} $N_M = \sum_x n_x$, \hspace{1cm} $N_{Dt} = \sum_x k_{x0}$

- Admissible configurations satisfy **Grassmann constraints**:

\[
n_x + \sum_{\pm \mu} k_{x\mu} \equiv 3
\]

- Configurations are generated using a **directed path (worm) algorithm**: very efficient, especially in the chiral limit. [Adams-Chandrasekharan '03]
Thermodynamics of $U(3)$ lattice QCD in the chiral limit

We work directly in the **chiral limit**: $m_q = 0 \iff N_M = 0$ (dimers only).

Thermodynamical quantities are derived from the partition function:

$$Z(\gamma) = \sum_{\{k\}} \left( \prod_{x,\mu} \frac{(3-k_{x\mu})!}{3!k_{x\mu}!} \right) \gamma^{2N_Dt}$$

which has the bare anisotropy coupling $\gamma$ as the only free parameter; the physical anisotropy is parameterized by $\xi(\gamma) = \frac{a}{a_t}$.

**Energy density:**

$$a^3a_t \varepsilon = -\frac{a^3a_t}{V} \left. \frac{\partial \log Z}{\partial T^{-1}} \right|_V = \frac{\xi}{\gamma} \frac{d\gamma}{d\xi} \langle 2n_{Dt} \rangle$$

**Pressure:**

$$a^3a_t p = a^3a_tT \left. \frac{\partial \log Z}{\partial V} \right|_T = \frac{\xi}{3\gamma} \frac{d\gamma}{d\xi} \langle 2n_{Dt} \rangle$$

**Interaction energy:** $\varepsilon - 3p = 0$

**Entropy density:** $s = \frac{4\varepsilon}{3T}$
Anisotropy calibration

Grassmann constraints imply locally conserved currents:

\[ j_{x \mu} = \sigma_x \left( k_{x \mu} - \frac{3}{8} \right) \Rightarrow \sum_{\pm \mu} (j_{x \mu} - j_{x-\mu}, \mu) = 0 \]

The variance of the associated conserved charges,

\[ j_\mu = \sum_{x \perp \mu} j_{x \mu} \]

should coincide in a hypercubic volume, and this provides a very precise method to calibrate the anisotropy, \( \xi(\gamma) = \frac{a}{a_t} \), with the help of multi-histogram reweighing:

\[ a_t N_t = a N_s \]

\[ \Downarrow \]

\[ \langle j_t^2 \rangle (\gamma_c) = \langle j_s^2 \rangle (\gamma_c) \]
Anisotropy calibration

Grassmann constraints imply locally **conserved currents**:

\[ \sum_{\mu} \left( j_{x\mu} - j_{x-\hat{\mu},\mu} \right) = 0 \]

The variance of the associated **conserved charges**,

\[ j_\mu = \sum_{x\perp \hat{\mu}} j_{x\mu} \]

should coincide in a hypercubic volume, and this provides a very precise method to calibrate the anisotropy, \( \xi(\gamma) = \frac{a}{a_t} \), with the help of multi-histogram reweighing:

\[ \xi(\gamma) \sim \gamma^2 \]

but the prefactor deviates from the mean field prediction \( (\xi = \gamma^2) \)
Running anisotropy

At the same time, the running anisotropy, \( \frac{d\xi}{d\gamma} \), can be computed directly from the critical value of \( \langle j^2 \rangle \), and the critical value of their slopes:

\[
\frac{d\gamma}{d\xi} = \frac{\langle j^2 \rangle_c}{\left( \frac{d}{d\gamma} \langle j^2_t \rangle - \frac{d}{d\gamma} \langle j^2_s \rangle \right)_{\gamma_c}}
\]
Energy density at $T = 0$

The $T = 0$ contribution must be carefully subtracted from the energy density:

$$a^4 \varepsilon_0(\xi) = \lim_{N_s \to \infty} \xi^2 \frac{d\gamma}{d\xi} \left(2n_{Dt}\right) \bigg|_{N_t = \xi N_s} \text{ (hypercubic)}$$

- Linear scaling, similar to the lattice gas of a free massless boson.

[Karsch-Engels-Satz '82]
Energy density at finite $T$

We take thermodynamic extrapolations ($N_s \to \infty$) of the energy density, normalized by $aT_c = 1.8843(1)$ [Forcrand-Unger '11], at fixed $\xi$ and $N_t$, assuming:

$$\frac{\epsilon(N_s, N_t, \xi) - \epsilon_0(\xi)}{T_c^4} = \frac{\epsilon(T) - \epsilon_0}{T_c^4} + \frac{c_1}{N_s^3} + \frac{c_2}{N_s^6} + \cdots$$

We use $N_s \gtrsim 2N_t$ and $\xi \geq 2$, for minimal lattice effects.
Energy density at finite $T$

...and after all extrapolations:

Preliminary fits are added for illustration:

$$
\frac{\epsilon(T) - \epsilon_0}{T_c^4} \approx c_2 \left( \frac{T}{T_c} \right)^2 + c_4 \left( \frac{T}{T_c} \right)^4 + c_6 \left( \frac{T}{T_c} \right)^6 + c_8 \left( \frac{T}{T_c} \right)^8 + \cdots
$$

- Near $T_c$: Repulsion between pions $\Rightarrow$ energy decreases
- At low $T$: Near-ideal gas of a single massless boson
- At very low $T$: $1/\xi$ corrections?
Energy density at finite $T$, in $SU(3)$ QCD

We perform the same study in $SU(3)$ QCD, for which there is a **monomer-dimer-loop** representation of the partition function, and for which the energy density receives **baryonic corrections**:

$$a^3 a_t \varepsilon = \mu_B \rho_B - \frac{a^3 a_t}{V} \frac{\partial \log Z}{\partial T} \bigg|_{V, \mu_B} = \frac{\xi}{\gamma} \frac{d\gamma}{d\xi} \langle 2n_D t + 3n_B t \rangle$$
Comparison between $U(3)$ and $SU(3)$

Near $T_c$:
- $U(3)$: Repulsion between pions $\Rightarrow$ energy decreases
- $SU(3)$: Energy is higher than in $U(3)$ due to baryonic modes

At low $T$: Pion gas is effectively free (up to $1/\xi$-corrections?)
- Qualitative consistency with mean field, at large-$N_c$
Summary and outlook

- In the strong coupling limit, \( U(N_c) \) lattice QCD with a massless staggered quark describes an ideal gas of massless pions, at low temperatures.

- We study the thermodynamics of \( N_f=1 \) \( U(3) \) and \( SU(3) \) lattice QCD, in the chiral and strong coupling limits, by simulating the dimer representation of this system with a directed path algorithm.

- We propose a prescription for a very precise renormalization of the bare anisotropy coupling, and for the determination of its running.

- We determine, with high precision, the dependence of the energy density on the temperature, thanks to an accurate subtraction of the \( T=0 \) contribution. In that regime, the system describes a near-ideal pion gas, just spoiled by massive modes near \( T_c \).

Next:

- Measure \( f_\pi^2 \), and compare with ChPT predictions.

- Extend the study of the equation of state of \( U(3) \) and \( SU(3) \) QCD to finite quark mass, finite baryon density, \( N_f > 1 \), etc.
Backup slides
Analytical integration over $U_{x\mu}$ and $\psi_x, \bar{\psi}_x$ in $SU(3)$ lattice QCD yields the partition function of a **monomer-dimer-loop system**: [Rossi-Wolff '84]

$$Z = \int \mathcal{D}U \mathcal{D}\psi \mathcal{D}\bar{\psi} \ e^{2a_t m_q \sum_x \bar{\psi}_x \psi_x + \sum_{x,\mu} \gamma^\delta_{\mu0} \eta_{x\mu} (e^{a_t \mu q} \bar{\psi}_x U_{x\mu} \psi_x + \bar{\psi}_x U_{x\mu} \psi_x + \bar{\psi}_x \psi_x)}$$

$$= \sum_{\{n, k, C\}} \frac{\sigma(C)}{N!|C|} \left( \prod_x \frac{3!}{n_x!} \right) \left( \prod_{x,\mu} \frac{(3 - k_{x\mu})!}{3!k_{x\mu}!} \right) (2a_t m_q)^{N_M} \gamma^{2N_D t + 3N_B t} e^{3N_t a_t \mu q \Omega(C)}$$

$n_x, k_{x\mu} \in \{0, 1, 2, 3\}$, \hspace{1cm} $N_D t = \sum_x k_{x0}$, \hspace{1cm} $N_M = \sum_x n_x$

$b_{x\mu} \in \{0, \pm 1\}$, \hspace{1cm} $N_B t = \sum_x |b_{x0}|$

- **Admissible configurations** satisfy **Grassmann constraints**:

  \[ n_x + \sum_{\pm \mu} k_{x\mu} = 3 \]

  \[ \sum_{x,\mu} |b_{x\mu}| = 0 \]

- **Baryonic sign problem**: $\sigma(C) = \pm 1$
Thermodynamics of $SU(3)$ lattice QCD

Thermodynamical quantities are derived from the partition function:

$$Z = \sum_{\{n, k, C\}} \sigma(C) \left( \prod_x \frac{3!}{n_x!} \right) \left( \prod_{x, \mu} \frac{(3 - k_x \mu)!}{3! k_x \mu!} \right) (2a_t m_q)^N \gamma^{2N_D t + 3N_B t} e^{3N_t a_t \mu_q \Omega(C)}$$

**Baryon number density:** \((\mu_B = 3\mu_q)\)

$$a^3 \rho_B = a^3 \frac{T}{V} \frac{\partial \log Z}{\partial \mu_B} \bigg|_{V,T} = \frac{\langle \Omega \rangle}{N_s^3} = \langle \omega \rangle$$

**Energy density:**

$$a^3 a_t \varepsilon = \mu_B \rho_B - \frac{a^3 a_t}{V} \frac{\partial \log Z}{\partial T^{-1}} \bigg|_{V, \mu_B} = \frac{\xi}{\gamma} \frac{d\gamma}{d\xi} \langle 2n_{Dt} + 3n_{Bt} \rangle - \langle n_M \rangle$$

**Pressure:**

$$a^3 a_t p = a^3 a_t T \frac{\partial \log Z}{\partial V} \bigg|_{T, \mu_B} = \frac{\xi}{3\gamma} \frac{d\gamma}{d\xi} \langle 2n_{Dt} + 3n_{Bt} \rangle$$

**Interaction energy:** \(\varepsilon - 3p = -\langle n_M \rangle\)

**Entropy density:**

$$s = \frac{1}{T} \left( \frac{4\varepsilon}{3} - \mu_B \rho_B \right)$$
Anisotropy calibration

In the chiral limit, the Grassmann constraints imply locally conserved currents:

\[ j_{x\mu} = \sigma_x \left( k_{x\mu} - \frac{3}{2} |b_{x\mu}| - \frac{3}{8} \right) \quad \implies \quad \sum_{\pm \mu} (j_{x\mu} - j_{x-\hat{\mu},\mu}) = 0 \]

The variances of the associated conserved charges, \( j_{\mu} = \sum_{x \perp \hat{\mu}} j_{x\mu} \) are used to calibrate the anisotropy, \( \xi(\gamma) = \frac{a}{a_t} \), just like in the \( U(3) \) case.

\[ \xi(\gamma) \sim \gamma^2 \]

but the prefactor again deviates from the mean field prediction \( (\xi = \gamma^2) \)
Energy density at $T = 0$ and $T > 0$

After subtracting the $T = 0$ contributions:

$$a^4\varepsilon_0(\xi) = \lim_{N_s \to \infty} \frac{\xi^2}{\gamma} \left. \frac{d\gamma}{d\xi} \langle 2n_D t + 3n_B t \rangle \right|_{N_t = \xi N_s} \text{ (hypercubic)}$$

we obtain a similar plot for the energy density at finite $T$, in units of the $SU(3)$ critical temperature: $aT_c = 1.402(2)$ [Forcrand-Langelage-Philipsen-Unger '14]
Measuring of the running anisotropy

The variances of the currents $j_{\mu}$ scale with the volume of lattice slices $\perp \hat{\mu}$:

$$\begin{align*}
\left\{ \langle j_t^2 \rangle &\propto a^3 \\
\langle j_s^2 \rangle &\propto a^2 a_t
\end{align*} \Rightarrow \frac{\langle j_t^2 \rangle}{\langle j_s^2 \rangle} = \frac{N_s}{N_t} \xi
$$

The derivative of this ratio wrt the bare anisotropy coupling, at the critical value $\gamma_c$, is related to the running of the anisotropy coupling:

$$\frac{d}{d\gamma} \left( \frac{\langle j_t^2 \rangle}{\langle j_s^2 \rangle} \right) \bigg|_{\gamma_c} = \frac{1}{\langle j^2 \rangle_c} \left( \frac{d}{d\gamma} \langle j_t^2 \rangle - \frac{d}{d\gamma} \langle j_s^2 \rangle \right) \bigg|_{\gamma_c} = \frac{N_s}{N_t} \frac{d\xi}{d\gamma} \bigg|_{\gamma_c} = \frac{1}{\xi} \frac{d\xi}{d\gamma} \bigg|_{\gamma_c}
$$

Inverting the relation above, we finally obtain:

$$\frac{d\gamma}{d\xi} = \frac{\langle j^2 \rangle_c}{\left( \frac{d}{d\gamma} \langle j_t^2 \rangle - \frac{d}{d\gamma} \langle j_s^2 \rangle \right) \bigg|_{\gamma_c}}$$