Non-perturbative anisotropy calibration in lattice QCD at strong coupling

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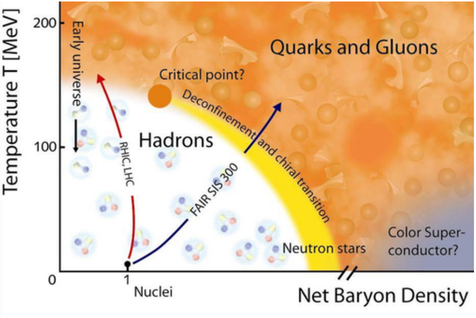
Motivation

- We want to understand QCD at **non-zero temperature** (T) and **non-zero chemical potential** (μ_q), from **first principles** $\Rightarrow$ **lattice QCD**.
- At $\mu_q \neq 0$, direct Monte Carlo simulations are impractical, due to the **sign problem**.



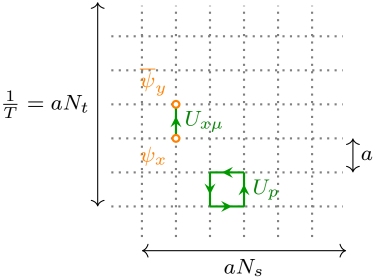
Outline

1. We review our approach for tackling the sign problem in the strong coupling limit: **diagrammatic QCD**, on anisotropic lattices.
2. We eliminate the main source of systematic errors by performing a precise, **non-perturbative anisotropy calibration**.

Lattice QCD

- We want to simulate QCD at **finite** T and **finite** μ_q, from first principles.
- Regularize QCD on an **Euclidian** $N_s^3 \times N_t$ **lattice**, with **spacing** a.
- The partition function of lattice QCD is a path integral over **link variables** $U_{x\mu} \in$ U(3) or SU(3) and $(N_f = 1)$ **staggered fermions** $\psi_x, \overline{\psi}_x$:

$$Z = \int \prod_{x,\mu} dU_{x\mu} \prod_x d\psi_x \, d\overline{\psi}_x \, e^{-S_g(U)} \, e^{-S_f(U,\overline{\psi},\psi)}$$



- The lattice is necessarily **bipartite**.
- **Finite temperature**: *pbc* on gauge fields, *apbc* on fermions.

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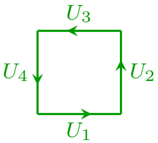
- **Wilson plaquette action**, with $\beta(a) = 6/g^2(a)$:

$$S_g(U) = \beta \sum_{\square} \left(1 - \frac{1}{3} \mathrm{ReTr}(U_1 U_2 U_3 U_4)\right)$$



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- **Staggered fermion action**, with $\eta_{x\mu} = \prod_\mu \gamma_\mu^{x_\mu} = (-1)^{\sum_{\nu<\mu} x_\nu}$, and with **quark chemical potential**, μ_q:

$$S_f(U,\overline{\psi},\psi) = -\sum_{x,\mu} \eta_{x\mu}(e^{a\mu_q}\overline{\psi}_x U_{x\mu}\psi_y - e^{-a\mu_q}\overline{\psi}_y U_{x\mu}^\dagger \psi_x) - 2am_q \sum_x \overline{\psi}_x \psi_x$$

Sign problem

- **Traditional approach** to simulating fermions: integrate $\psi, \overline{\psi}$, sample over U:

$$Z = \int dU\, d\psi\, d\overline{\psi}\, e^{-S_g(U) - S_f(U,\psi,\overline{\psi})} = \int dU\, e^{-S_g(U)} \det\left(\not{D}_U(m_q) + \mu_q \gamma_0\right)$$

- The quark chemical potential breaks C-symmetry when $\mathrm{Re}(\mu_q) \neq 0$:
complex measure $\Rightarrow$ sign problem

$$\det\left(\not{D}_U(m_q) + \mu_q \gamma_0\right)^* = \det\left(\not{D}_U(m_q) - \mu_q^* \gamma_0\right) \in \mathbb{C}$$

- **Reweighting:** The signal degrades exponentially with the volume V:

$$\langle \mathrm{sign} \rangle = Z/Z_+ \sim e^{-V \Delta f}$$

$V \Delta f$ measures the free energy barrier between the **true ensemble**, Z, and the **reweighed ensemble**, Z_+, *i.e.* the **severity of the sign problem**.
In the traditional approach, $\Delta f \sim O(1)$.

Sign problem

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- Popular methods for tackling the sign problem in QCD:
  - Analytical continuation (from imaginary μ_q)
  - Complex Langevin
  - Lefschetz thimbles
  - Density of states method
  - Diagrammatic approach ("dual variables")
  - ...

- We use the **diagrammatic approach**!

Sign problem

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- **Problem:** U fluctuates $\Rightarrow$ det $\not{D}_U$ fluctuates $\Rightarrow$ sign problem.

- **Alternative approach (diagrammatic):** Reverse the order of integration!
  1. Integrate U $\Rightarrow$ fermionic color singlets
  2. Integrate $\psi, \overline{\psi}$ $\Rightarrow$ diagrams

- Why is it a good idea?
  - The sign problem is **representation-dependent**, *e.g.* in the eigenbasis of $\widehat{H}$, transfer matrix elements are positive-definite $\Rightarrow$ no sign problem.
  - Fermionic **color singlets** are closer to the physical eigenstates of QCD than the (colored) link states.

- The hope is that the sign problem of QCD, in the new representation, becomes **sufficiently mild** to allow for reweighting.

Diagrammatic QCD

- Take the **strong coupling limit** ($\beta = 0$): the partition function **factorizes** into a product of solvable **one-link integrals**, $I_{x\mu}$:

$$Z = \int d\psi\, d\overline{\psi}\, e^{2am_q \sum_x M_x} \prod_{x,\mu} \underbrace{\int dU_{x\mu}\, e^{\eta_{x\mu}\left(e^{a\mu_q}\overline{\psi}_x U_{x\mu}\psi_{x+\hat{\mu}} - e^{-a\mu_q}\overline{\psi}_{x+\hat{\mu}} U_{x\mu}\psi_x\right)}}_{I_{x\mu}}$$

- Integration over U generates terms with fermionic **color singlets**: [Rossi & Wolff '84]

$$I_{x\mu} = \sum_{k=0}^{3} \left\{ \frac{(3-k)!}{3!k!} (M_x M_{x+\hat{\mu}})^k \underbrace{+ \frac{\eta_{x\mu}}{3!} \left(e^{3a\mu_q} \bar{B}_x B_{x+\hat{\mu}} - e^{-3a\mu_q} \bar{B}_{x+\hat{\mu}} B_x\right)}_{\mathrm{SU}(3)} \right\}$$

where $M_x = \overline{\psi}_x \psi_x$ **(meson)** and $B_x = \frac{1}{3!}\varepsilon_{ijk}\psi_x^i \psi_x^j \psi_x^k$ **(baryon)**.

- Further integration over $\psi, \overline{\psi}$ yields a combinatorial partition function, with constraints.

Diagrammatic QCD

- Integration over $\psi, \overline{\psi}$ yields a **monomer-dimer-loop** ensemble: [Rossi & Wolff '84]

$$Z = \sum_{\{n,k,\ell\}} \mathcal{C}\{n,k,\ell\} \prod_{x,\mu} \frac{(3-k_{x\mu})!}{3!k_{x\mu}!} \prod_x \frac{3!}{n_x!} (2am_q)^{N_M} \underbrace{\frac{\sigma(\ell)}{3!^{|\ell|}} e^{3w_\ell \mu_q/T}}_{\mathrm{SU}(3)}$$

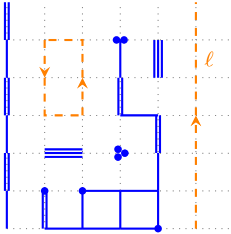
$$N_M = \sum_x n_x, \qquad \sigma(\ell) = \pm 1, \qquad w_\ell = \text{baryon winding}$$

- **Grassmann constraints**:

$$\mathcal{C}\{n,k,\ell\} = \prod_x \delta\left(n_x + \sum_{\pm\mu} k_{x\mu} - 3\right) \underbrace{\delta\left(\sum_{\pm\mu} \ell_{x\mu}\right)}_{\mathrm{SU}(3)}$$

- **Degrees of freedom** are integer occupation numbers of **monomers** (n_x), **dimers** $(k_{x\mu})$, and **baryon links** $(\ell_{x\mu})$:

x ●	$(M_x)^{n_x}$	$n_x \in \{0,1,2,3\}$
x —— y	$(M_x M_y)^{k_{xy}}$	$k_{xy} \in \{0,1,2,3\}$
x - - → - - y	$-\overline{B}_y B_x$	$\ell_{xy} \in \{0, \pm 1\}$
x - - ← - - y	$\overline{B}_x B_y$	



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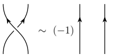
- **Observables**:

$$\langle \overline{\psi}\psi \rangle = \frac{\langle n_M \rangle}{2am_q}, \qquad \chi = \langle \overline{\psi}\psi\overline{\psi}\psi \rangle = \sum_{\text{worms}} 1, \qquad \text{etc.}$$

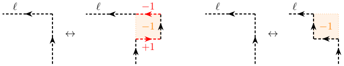
- The **sign problem** comes from baryon loops:

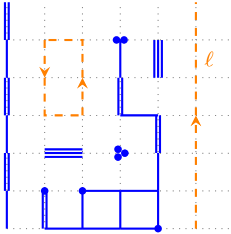
$$\sigma(\ell) = (-1)^{w_\ell + 1} (-1)^{N_{\ell-}} \prod_{l \in \ell} \eta_l$$

Topological



Geometric





Worm algorithm

- **Directed-path algorithms** propagate a local violation of the Grassmann constraints along a **worm**. [Adams & Chandrasekharan '03]
- A worm has a **head** (○) and a **tail** (●).
- **Updating algorithm:**
  1. **Violate** constraints + detailed balance on starting site (head = tail);
  2. Propagate the head, by alternating local **active/passive updates** (local detailed balance is satisfied)
     $\Rightarrow$ samples the **2-pt function**: $\langle \overline{\psi}_{\circ} \psi_{\circ} \overline{\psi}_{\bullet} \psi_{\bullet} \rangle$
  3. Restore detailed balance + constraints (globally) when head = tail
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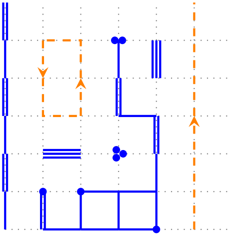

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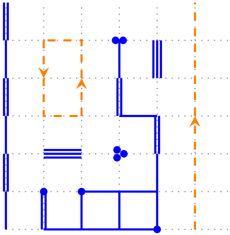

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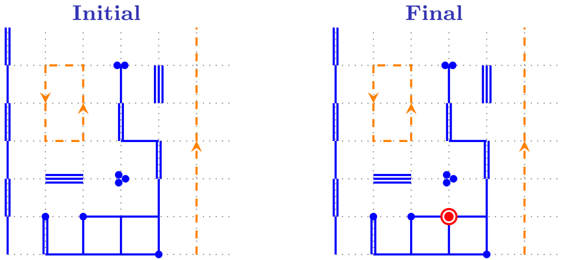

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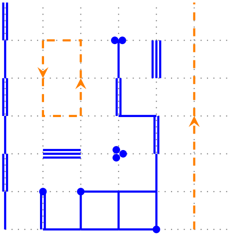

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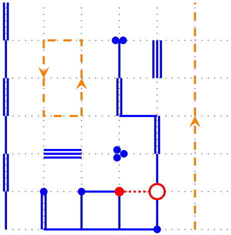

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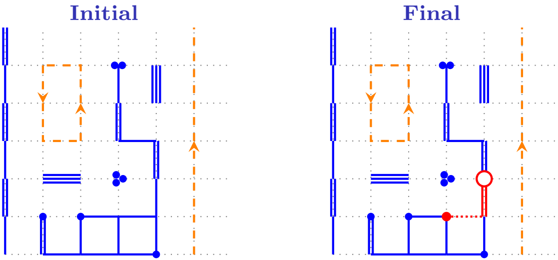

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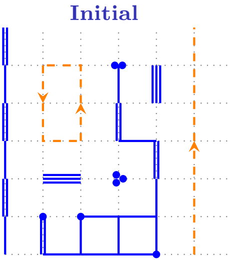

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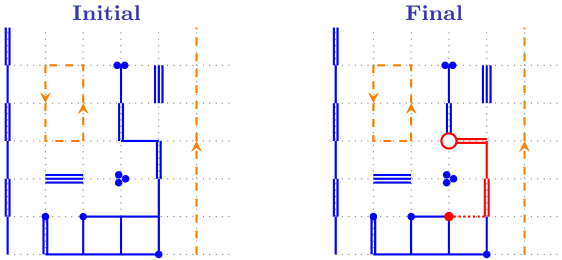

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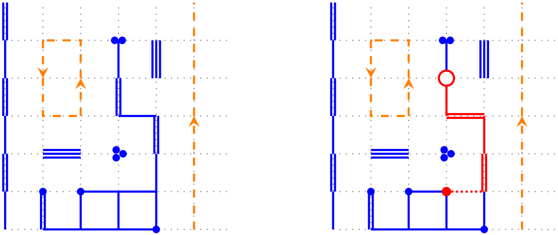

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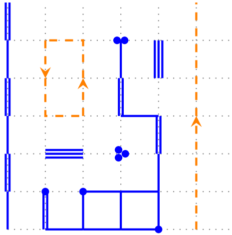

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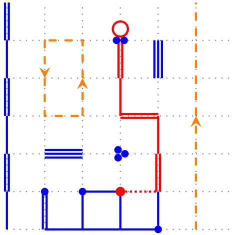

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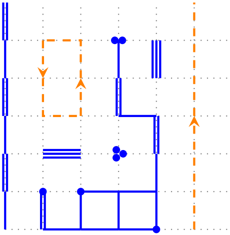

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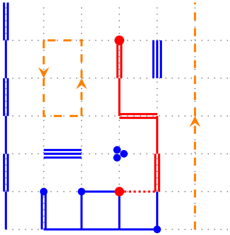

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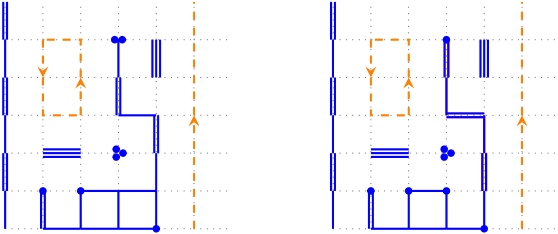


- A **baryonic worm** replaces:  $\leftrightarrow$ 

Lattice anisotropy

- **Problem:** The critical temperature of the chiral phase transition in QCD, at $\beta = 0$, is too high: [Forcrand, Langelage, Philipsen & Unger '14]

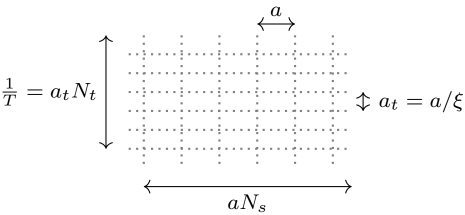
$$aT_c = 1.402(2) > \frac{1}{2}$$

i.e. it is inaccessible, even taking the smallest possible $N_t = 2$.

- **Solution:** Use independent lattice spacings (a, a_t), characterized by the physical anisotropy parameter ξ [Engels, Karsch, Satz & Montvay '82]

$$\xi = \frac{a}{a_t}$$

- Allows independent limits: continuous time, thermodynamic
- Allows continuous tuning of $aT = \frac{\xi}{N_t}$



Lattice anisotropy

The anisotropy enters the lattice action in the form of a **bare coupling** γ:

$$S_g = \beta \sum_x \left[\frac{1}{\gamma} \sum_{i<j} \left(1 - \frac{1}{3} \mathrm{ReTr}\,(U_{xij}) \right) + \gamma \sum_i \left(1 - \frac{1}{3} \mathrm{ReTr}\,(U_{xi0}) \right) \right]$$

$$S_f = -2 a_t m_q \sum_x \overline{\psi}_x \psi_x - \sum_{x,\mu} \eta_{x\mu} \gamma^{\delta_{\mu 0}} (e^{a_t \mu_q} \overline{\psi}_x U_{x\mu} \psi_y - e^{-a_t \mu_q} \overline{\psi}_y U^{\dagger}_{x\mu} \psi_x)$$

which needs to be renormalized: $\xi \equiv \xi(\gamma)$

Renormalization prescriptions:

- Perturbative ($\beta \gg 1$): [Karsch '82; Karsch & Stamanescu '89]

$$\xi(\gamma) \approx \gamma + O(\beta^{-1})$$

- Mean-field ($\gamma \gg 1$): [Faldt & Petersson '86; Bilic, Karsch & Redlich '92]

$$\xi(\gamma) \approx \gamma^2$$

- Non-perturbative [Levkova & Manke '02; Nomura, Ueda & Matsufuru '04 '05]

Lattice anisotropy

The anisotropy enters the lattice action in the form of a **bare coupling** γ:

$$S_g = \beta \sum_x \left[\frac{1}{\gamma} \sum_{i<j} \left(1 - \frac{1}{3} \mathrm{ReTr}\,(U_{xij}) \right) + \gamma \sum_i \left(1 - \frac{1}{3} \mathrm{ReTr}\,(U_{xi0}) \right) \right]$$

$$S_f = -2a_t m_q \sum_x \overline{\psi}_x \psi_x - \sum_{x,\mu} \eta_{x\mu} \gamma^{\delta_{\mu 0}} (e^{a_t \mu_q} \overline{\psi}_x U_{x\mu} \psi_y - e^{-a_t \mu_q} \overline{\psi}_y U^\dagger_{x\mu} \psi_x)$$

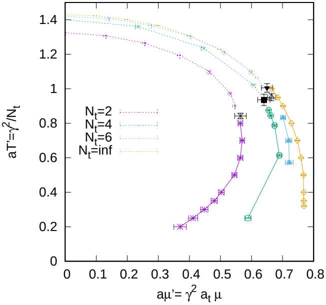
Diagrammatic QCD on anisotropic lattices (at $\beta = 0$):

$$Z = \sum_{\{n,k,\ell\}} \left(\prod_x \frac{3!}{n_x!} \right) \left(\prod_{x,\mu} \frac{(3-k_{x\mu})!}{3! k_{x\mu}!} \right) (2a_t m_q)^{N_M} \gamma^{2N_{Dt}} \underbrace{{}^{+3N_{\ell t}} \frac{\sigma(\ell)}{3!^{|\ell|}} e^{3 w_\ell \mu_q / T}}_{\mathrm{SU}(3)}$$

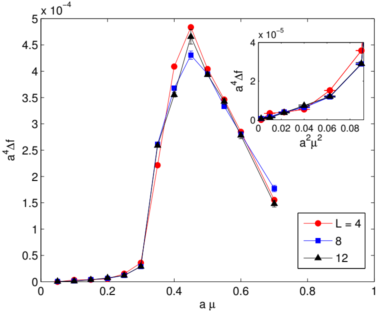
$$N_M = \sum_x n_x, \qquad N_{Dt} = \sum_x k_{x0}, \qquad N_{\ell t} = \sum_x |\ell_{x0}|$$

Phase diagram at $\beta = 0$

- One **phase boundary** separates a chirally broken phase at low (T, μ_q), from a chirally symmetric phase at high (T, μ_q).
- Phase boundaries $aT_c(a\mu_q)$ computed for $N_t = 2, 4, 6$, using **mean-field** $\xi(\gamma)$ $\Rightarrow$ strong dependence on N_t.
- The sign problem is **mild:** $\Delta f \sim O(10^{-4})$.



[Forcrand & Fromm '09]



- The mean-field prescription for ξ is a **systematic error**.
- We propose a **non-perturbative prescription**.

Conserved currents and charges

Take the **Grassmann constraints**:

$$\begin{cases} (\psi_x)^3: & n_x + \sum_{\pm\mu} \left(k_{x\mu} + 3\,\Theta(+\ell_{x\mu})\right) = 3 \\ (\overline{\psi}_x)^3: & n_x + \sum_{\pm\mu} \left(k_{x\mu} + 3\,\Theta(-\ell_{x\mu})\right) = 3 \end{cases}$$

Adding the two constraints yields:

$$\sum_{\pm\mu} \left(k_{x\mu} + \frac{3}{2}|\ell_{x\mu}| - \frac{3}{8} \right) = -n_x$$

Then, we may define discrete **pion currents**: [Chandrasekharan & Strouthos '03]

$$j_{x\mu} \stackrel{\text{def}}{=} \sigma_x \left(k_{x\mu} + \frac{3}{2}|\ell_{x\mu}| - \frac{3}{8} \right) \quad \Rightarrow \quad \sum_{\mu=0}^{3} \left(j_{x\mu} - j_{x-\hat{\mu},\mu} \right) = -\sigma_x n_x$$

$$\sigma_x = (-1)^{\sum_\nu x_\nu} = \text{parity of site } x$$

Monomers are sources $\Rightarrow$ $j_{x\mu}$ are **conserved in the chiral limit** ($am_q = 0$).

Conserved currents and charges

- **In the chiral limit**, the pion currents are conserved:

$$j_{x\mu} \overset{\text{def}}{=} \sigma_x \left(k_{x\mu} + \frac{3}{2}|\ell_{x\mu}| - \frac{3}{8} \right)$$

  and so are the corresponding **pion charges** (**helicity moduli**), defined over a codim-1 lattice slice $\mathcal{S}_\mu$, perpendicular to $\hat{\mu}$:

$$Q_\mu \overset{\text{def}}{=} \sum_{x \in \mathcal{S}_\mu} j_{x\mu}$$

- Q_μ measures the **winding of meson loops** of a given configuration, around the $\hat{\mu}$-direction.
- $\langle Q_\mu \rangle = 0$, from parity symmetry.
- On an isotropic lattice, its variance is related to the **pion decay constant**: [Hasenfratz & Leutwyler '90, Chandrasekharan & Jiang '03]

$$F_\pi^2 = \lim_{N_s \to \infty} \frac{1}{N_s^2} \langle Q^2 \rangle$$

Renormalised anisotropy

Consider the fluctuations of the timelike and spacelike pion charges:

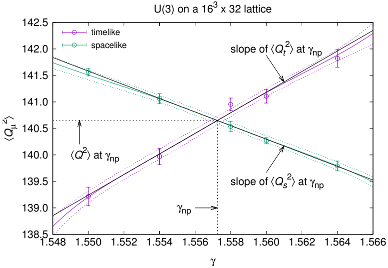
$$Q_t^2 \stackrel{\text{def}}{=} Q_0^2 \qquad\qquad Q_s^2 \stackrel{\text{def}}{=} \frac{1}{3}\sum_{i=1}^{3} Q_i^2$$

Renormalization criterion: Pion charge fluctuations must the same in all directions, on a hypercubic volume: [Forcrand, HV, Romatschke & Unger '16]

$$\langle Q_t^2\rangle_{\gamma_{\rm np}} = \langle Q_s^2\rangle_{\gamma_{\rm np}} \;\Rightarrow\; a_t N_t = a N_s \;\Rightarrow\; \xi(\gamma_{\rm np}) = \frac{N_t}{N_s}$$

Procedure:

1. Select the target anisotropy $a/a_t = \xi$ on a $N_s^3 \times (\xi N_s)$ lattice.
2. Tune γ until $\langle Q_t^2\rangle_\gamma = \langle Q_s^2\rangle_\gamma$ (use multi-histogram reweighting).
3. Take $\xi(\gamma) = N_t/N_s$.



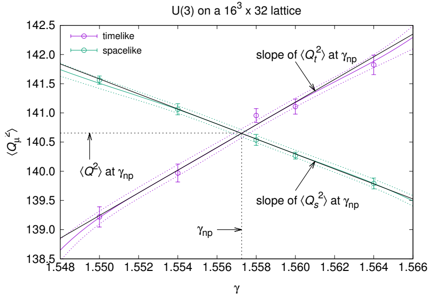
Running anisotropy

We also estimate the non-perturbative analogue of **Karsch's coefficients**:
[Karsch '82; Karsch & Stamanescu '89]

$$\frac{d\xi}{d\gamma}$$

It is necessary for the computation of bulk thermodynamic quantities, *e.g.* the **energy density**:

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



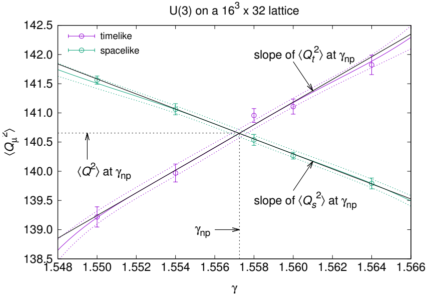
Running anisotropy

The variances of the conserved charges scale with the volume of slices $\mathcal{S}_\mu$:

$$\begin{cases} \langle Q_t^2 \rangle \propto (N_s a)^3 \\ \langle Q_s^2 \rangle \propto (N_s a)^2 N_t a_t \end{cases} \quad \Rightarrow \quad \frac{\langle Q_t^2 \rangle}{\langle Q_s^2 \rangle} = \frac{N_s}{N_t} \xi$$

The derivative of this ratio wrt γ, at $\gamma_{\rm np}$, is related to the running of ξ:

$$\frac{1}{\xi} \frac{d\xi}{d\gamma}\bigg|_{\gamma_{\rm np}} = \frac{N_s}{N_t} \frac{d\xi}{d\gamma}\bigg|_{\gamma_{\rm np}} = \frac{d}{d\gamma} \frac{\langle Q_t^2 \rangle}{\langle Q_s^2 \rangle}\bigg|_{\gamma_{\rm np}} = \frac{\langle Q_t^2 \rangle'_{\gamma_{\rm np}} - \langle Q_s^2 \rangle'_{\gamma_{\rm np}}}{\langle Q^2 \rangle_{\gamma_{\rm np}}}$$



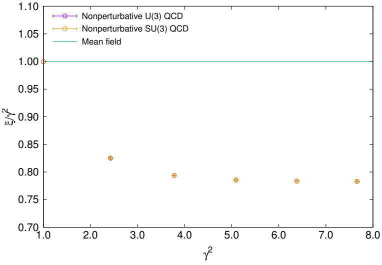
Non-perturbative vs. mean-field

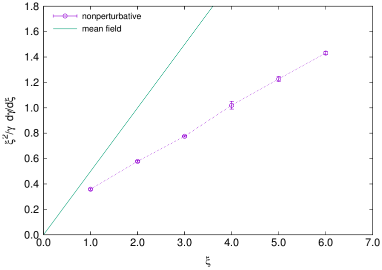
- Large non-perturbative corrections, $\delta \sim O(30\%)$, to the prefactor of the mean-field renormalised anisotropy:

$$\xi \sim (1+\delta)\,\gamma^2$$

and to its derivative:

$$\frac{d\xi}{d\gamma} \sim (1+\delta)\,2\gamma$$

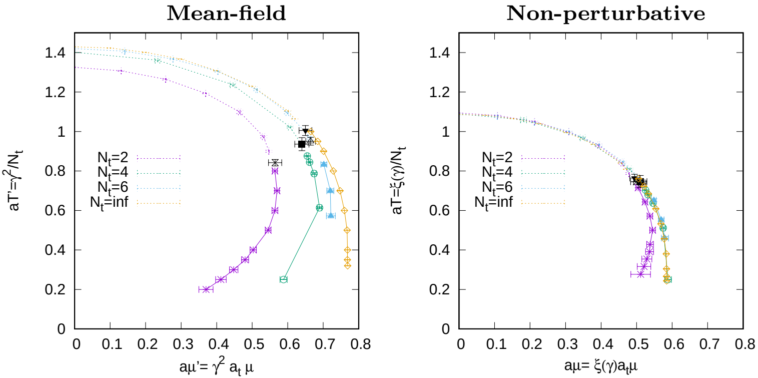




- The large correction affects observables significantly.

Phase diagram at $\beta = 0$

- The non-perturbative prescription for ξ reduces the N_t-dependence significantly $\Rightarrow$ very close to the continuous time limit.
- $aT_c(\mu_q = 0)$ and $a\mu_{q,c}(T = 0)$ decrease by $O(30\%)$.

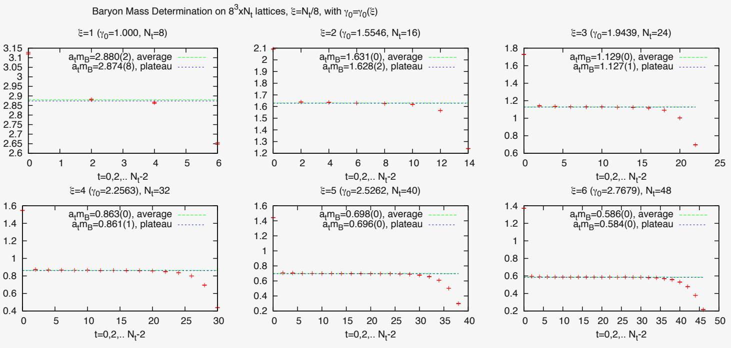


Baryon mass

- Determine the static baryon mass using the **snake algorithm**: [Forcrand, d'Elia & Pepe '00]

$$a m_B = \frac{\xi}{N_t} \sum_{k=0}^{N_t-2} \log \frac{Z_{k+2}}{Z_k}$$

It measures the cost in free energy of extending an open baryon segment of length k to a nearest site (of the same parity).

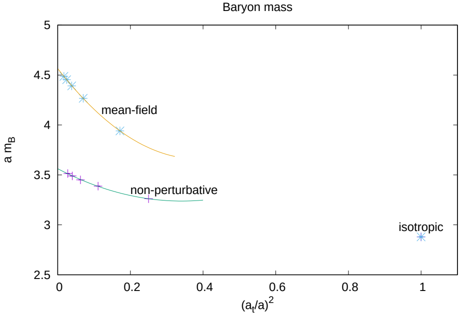


Baryon mass

- Determine the static baryon mass using the **snake algorithm**: [Forcrand, d'Elia & Pepe '00]

$$am_B = \frac{\xi}{N_t} \sum_{k=0}^{N_t-2} \log \frac{Z_{k+2}}{Z_k}$$

- The baryon mass changes with anisotropy by $\sim 50\%$ with the mean-field prescription, and only by $\sim 20\%$ with the non-perturbative prescription.



Summary

- The sign problem is “solved” in lattice QCD with staggered fermions, at $\beta = 0$.
- We propose a very precise non-perturbative renormalization of the lattice anisotropy at $\beta = 0, a_t m_q = 0$, using conserved charges.
- We observe large corrections to the mean-field prescrition.
- The systematic errors are significantly reduced using the new prescription.

Outlook

- To extend the non-perturbative prescription to:

  1. $a_t m_q > 0$
  2. $\beta > 0$