Towards a Dual Representation of Lattice QCD

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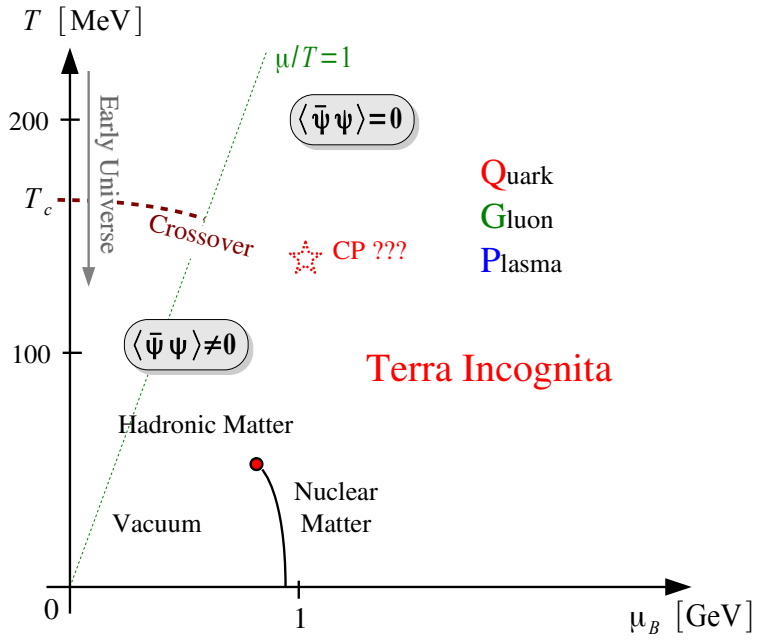
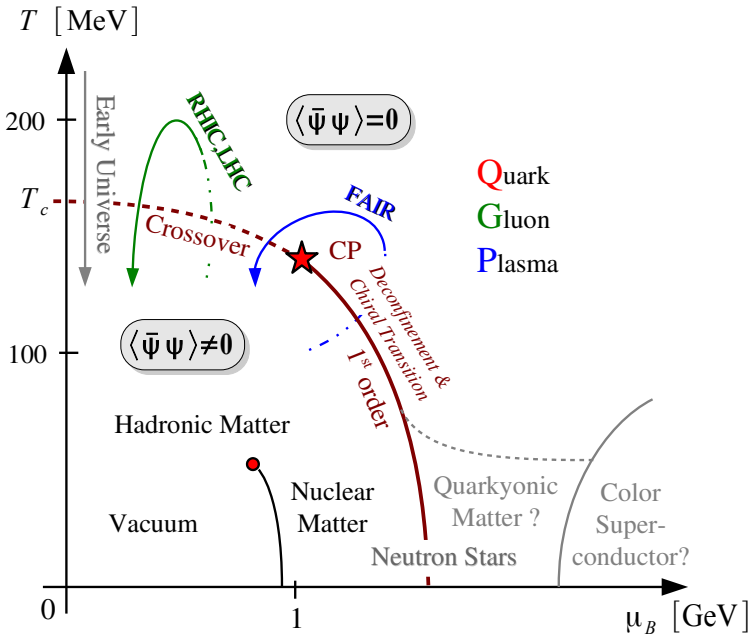
Sign Workshop 2018, Bielefeld

Motivations

Why to use dual representations for finite density lattice QCD?

QCD at finite density





- Simulations at finite μ_B in the standard determinantal approach hindered by the **sign problem**. A lot of open questions:
  - Existence/Location of the critical point.
  - Nature of the cold and dense phase (CFL colour superconductor?).
  - Silver blaze.

Sign problem is **representation dependent**!
$\Longrightarrow$ dual representations can tame it!

Overview of the available dual formulations

Pure Yang-Mills theory:

- Alternative formulation for $SU(3)$ using Hubbard Stratonovich transformation: [H. Vairinhos & P. De Forcrand '14]
- Plaquette expansion for pure Yang-Mills SU(2) gauge theory: [Leme, Oliveira,Krein '17]

Dual formulations with matter fields:

- Nuclear Physics from lattice QCD at strong coupling: [P. De Forcrand & M. Fromm '09]
- Dual lattice simulation of the U(1) gauge-Higgs model at finite density: [Mercado, Gattringer, Schmidt '13]
- Dual simulation of the massless lattice Schwinger model with topological term and non-zero chemical potential: [Göschl '17]
- Abelian color cycles (**ACC**): [Gattringer & Marchis '17]
- Dual $U(N)$ LGT with staggered fermions: [Borisenko et al '17]

Strong Coupling expansion: definition and motivations

- Strong coupling expansion is a, brute force, Taylor expansion of the **gauge action** in the lattice gauge coupling $\beta = \frac{2N_c}{g^2}$.

$$Z = \int d\chi_x d\bar{\chi}_x \prod_\ell \int_G dU_\ell e^{\sum_p \frac{\beta}{N_c} \mathrm{Re}(\mathrm{Tr} U_p)} \cdot e^{\mathrm{Tr}\left[U_\ell \mathcal{M}_\ell^\dagger + U_\ell^\dagger \mathcal{M}_\ell\right]}$$

$$= \int d\chi_x d\bar{\chi}_x \sum_{\{n_p, \bar{n}_p\}} \prod_{\ell,p} \frac{(\beta/2N_c)^{n_p+\bar{n}_p}}{n_p! \bar{n}_p!} \int_G dU_\ell \mathrm{Tr}[U_p]^{n_p} \mathrm{Tr}[U_p^\dagger]^{\bar{n}_p} e^{\mathrm{Tr}\left[U_\ell \mathcal{M}_\ell^\dagger + U_\ell^\dagger \mathcal{M}_\ell\right]}$$

Strong Coupling Limit: $\beta = \frac{2N_c}{g^2} \to 0$

- Gauge fields can be **integrated out**!
- Dual representation via **color singlets**.
- Sampling using Worm algorithms.

$$Z_{sc} = \int [dU] \int d\chi \bar{\chi} \; e^{-(\cancel{S_g} + S_f)}$$

The strong coupling partition function

- The **1-link** integral can be performed analytically

$$J_0[\mathcal{M},\mathcal{M}^\dagger] = \int_G dU e^{\mathrm{Tr}[U\mathcal{M}^\dagger + \mathcal{M}^\dagger U]}$$

- After Grassman integration ($N_f = 1$,staggered fermions):

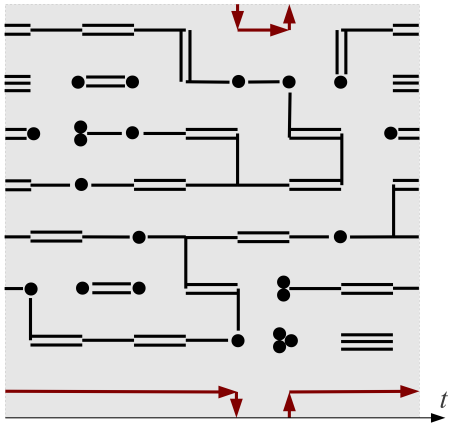
$$Z_{SC}(m_q,\mu) = \sum_{\{k,n,\ell\}} \underbrace{\prod_{b=(x,\mu)} \frac{(N_c-k_b)!}{N_c!k_b!}}_{\text{meson hoppings } M_x M_y} \underbrace{\prod_x \frac{N_c!}{n_x!}(2am_q)^{n_x}}_{\text{chiral cond. } \bar{\chi}\chi} \underbrace{\prod_\ell w(\ell,\mu)}_{\text{baryon hoppings } \bar{B}_x B_y}$$

$k_b \in \{0,\dots N_c\}$, $n_x \in \{0,\dots N_c\}$, $\ell_b \in \{0,\pm 1\}$, QCD: $N_c = 3$ [Wolff & Rossi, 1984]

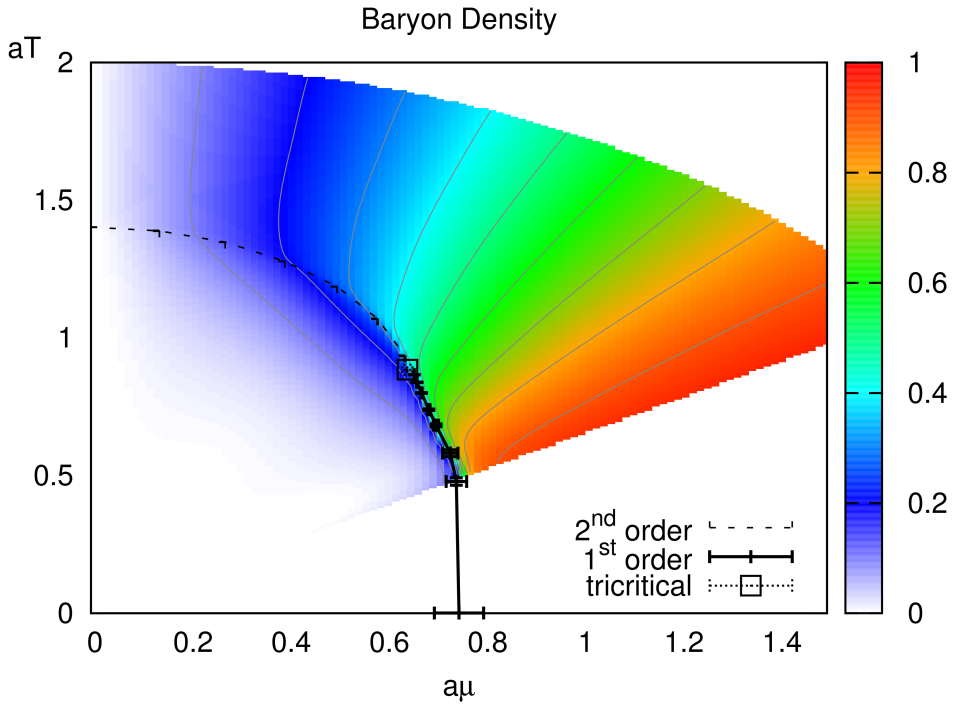
- **Grassman constraint**:

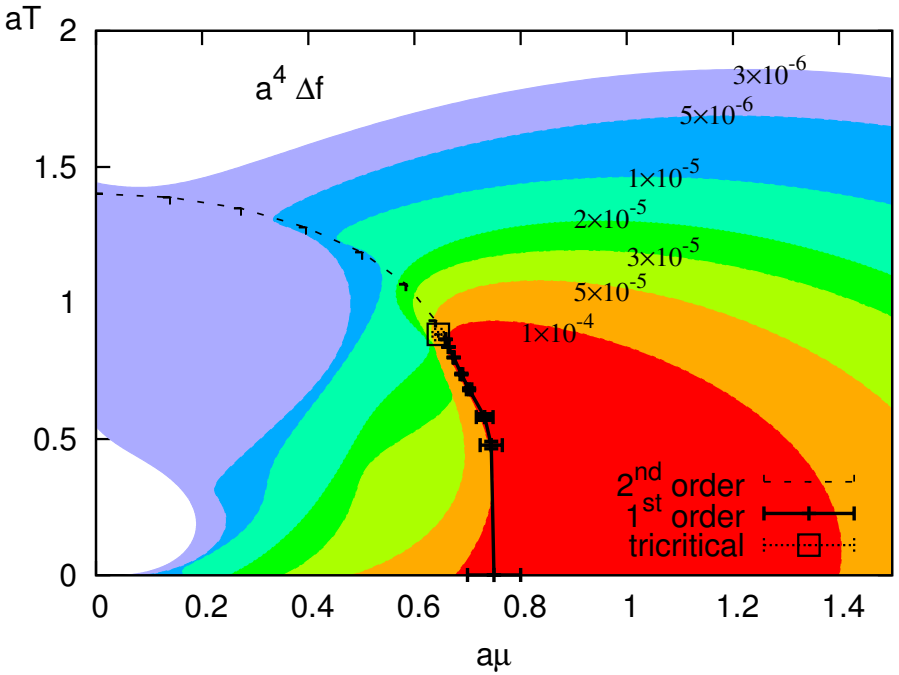
$$n_x + \sum_{\pm\mu}\left(k_\mu(x) + \frac{N_c}{2}|\ell_\mu(x)|\right) = N_c$$

- Residual sign problem in $w(\ell,\mu)$.



Strong coupling QCD





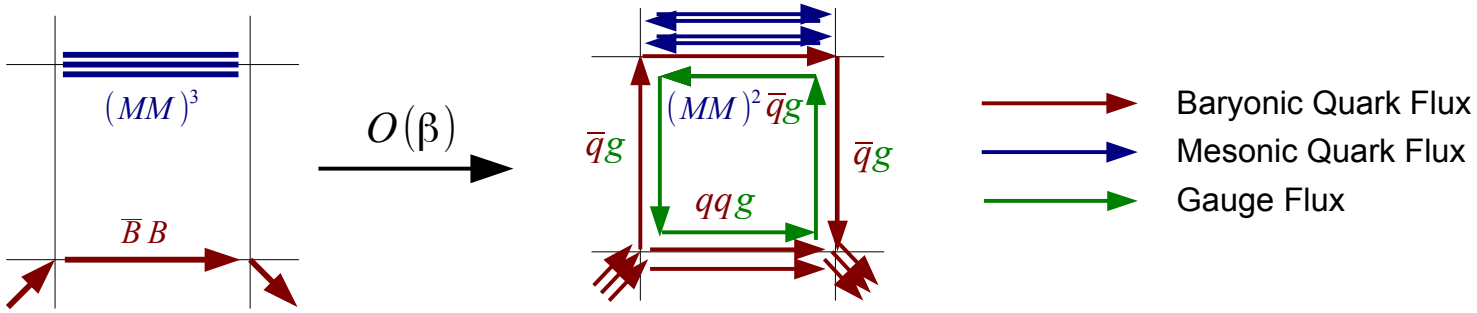
Advantages:

- Average complex phase $\langle e^{i\phi} \rangle_{pq} = e^{-\frac{V}{T}(f_{pq} - f)}$ close to one.
  $\Longrightarrow$ **sign problem** is mild and **phase diagram** can be mapped out.
- Simulations are fast and no supercomputers are required.
- Chiral limit even faster than the massive case.

Con: Lattice is maximally coarse.

Going beyond strong coupling QCD

- At $\beta = 0$ just color singlets **[mesons & baryons]**
  $\Longrightarrow$ **MDP formulation**.
- β corrections to strong coupling needed to make the lattice finer. Plaquette excitations produce **world sheets** bounded by **quark fluxes**:



- Gauge integrals become **strongly coupled** at $\beta > 0$.

Caveat: Dual representation does not solve, *per sè*, the sign problem. Plaquette contributions **could** reintroduce it.

Revisiting Link Integration for $SU(N)$

One-Link Integrals

- Link Integrals **no longer factorizes** in presence of plaquettes.
- The 1-link integrals must be now computed explicitly with **open color indices**. Example at $O(\beta)$:

$$\prod_\ell \int dU_\ell e^{\frac{\beta}{2N_c}\mathrm{Tr}[U_p+U_p^\dagger]} \cdot e^{\mathrm{Tr}\left[U_\ell \mathcal{M}_\ell^\dagger + U_\ell^\dagger \mathcal{M}_\ell\right]} \approx$$

$$\prod_\ell \int dU_\ell (1 + \underbrace{\frac{\beta}{2N_c}\mathrm{Tr}[U_p + U_p^\dagger]}_{O(\beta)\text{correction}}) \cdot e^{\mathrm{Tr}\left[U_\ell \mathcal{M}_\ell^\dagger + U_\ell^\dagger \mathcal{M}_\ell\right]}$$

- After the **hopping expansion** of the fermionic action:

$$\prod_{\ell\in p} \int dU_\ell \frac{\beta}{2N_c}\mathrm{Tr}[U_p] e^{\mathrm{Tr}\left[U_\ell \mathcal{M}_\ell^\dagger + U_\ell^\dagger \mathcal{M}_\ell\right]} = \mathrm{Tr}[\prod_{\ell\in p} J_\ell]$$

$$(J_\ell[\mathcal{M},\mathcal{M}^\dagger])^n_m = \sum_{\kappa_\ell,\bar\kappa_\ell} \frac{1}{\kappa_\ell!\bar\kappa_\ell!} \prod_{\alpha=1}^{\kappa_\ell} (\mathcal{M}_\ell)^{i_\alpha}_{j_\alpha} \prod_{\beta=1}^{\bar\kappa_\ell} (\mathcal{M}_\ell^\dagger)^{k_\beta}_{\ell_\beta} \underbrace{\mathcal{I}^{k_\ell+1,\bar k_\ell}_{m+\boldsymbol{i}\; n+\boldsymbol{j},\boldsymbol{k}\;\ell}}_{\text{Gauge integral to compute}}$$

One-Link Integrals

The prototype of Gauge Integral to compute is:

$$\mathcal{I}^{a,b}_{\boldsymbol{i}\boldsymbol{j},\boldsymbol{k}\ell} = \int_{SU(N_c)} dU \prod_{\alpha=1}^{a} U^{j_\alpha}_{i_\alpha} \prod_{\beta=1}^{b} (U^\dagger)^{\ell_\beta}_{k_\beta} \qquad \mid a-b \mid = q \cdot N_c$$

- Cases $a = 0$ and $q = 0, 1$ addressed: [Creutz 1978, Collins '03,'06, Zuber '17].
- We extended their results by computing the **generating functional**:

$$Z^{a,b}[K,J] = \int_{SU(N)} dU \big[\mathrm{Tr}(UK)\big]^a \big[\mathrm{Tr}(U^\dagger J)\big]^b$$

$$\overset{n=\min\{a,b\}}{=} (qN_c+n)! \underbrace{\prod_{i=0}^{N_c-1} \frac{i!}{(i+q)!} (\det K)^q}_{\textbf{Baryonic contrib.}} \underbrace{\sum_{\rho\vdash n} \tilde{W}^{n,q}_g(\rho, N_c) t_\rho(JK)}_{\textbf{Mesonic contrib.}}$$

$$\tilde{W}^{n,q}_g(\rho, N_c) = \sum_{\substack{\lambda\vdash n \\ \ell(\lambda)\leq N_c}} \frac{1}{(n!)^2} \frac{f_\lambda^2 \chi^\lambda(\rho)}{D_{\lambda, N_c+q}}, \qquad t_\rho(A) = \prod_{\rho_i} \mathrm{Tr}(A^{\rho_i})$$

One-Link Integrals: The Weingarten functions

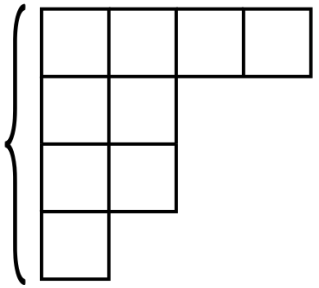
$Z^{a,b}[K,J]$ expressed as a sum over integer partitions weighted by the **modified Weingarten functions** $\tilde{W}_g$.

- Group theoretical factors enter the expression for $\tilde{W}_g^{n,q}$: $f_\lambda, D_{\lambda,N}$ dimensions of irrep λ of S_n and $SU(N_c)$. $\chi^\lambda(\rho)$ are the **irreducible characters** of the symmetric group.
- $\tilde{W}_g^{n,q}$ take as an argument both N_c and ρ. **Conjugacy classes of permutations** can also be represented as integer partitions.

$$\tilde{W}_g^{n,q}(\rho, N_c) = \sum_{\substack{\lambda \vdash n \\ \ell(\lambda) \leq N_c}} \frac{1}{(n!)^2} \frac{f_\lambda^2 \chi^\lambda(\rho)}{D_{\lambda, N_c+q}}$$

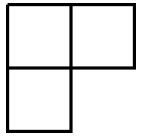
$\lambda \vdash 9 = (4,2,2,1)$

$\ell(\lambda) = 4$



$\lambda_1 = 4$
$\lambda_2 = 2$
$\lambda_3 = 2$
$\lambda_4 = 1$

$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 1 & 3 \end{pmatrix} \cong (12)(3) \cong$$



$\mathcal{I}^{a,b}$ obtained from $Z^{a,b}[K,J]$ by differentiating in J, K.

Application to Strong Coupling QCD with $O(\beta)$ correction

$O(\beta)$ Corrections: Derivation

Relevant gauge integrals at $O(\beta)$:

$$\mathcal{I}^{n,n}_{\boldsymbol{i}\boldsymbol{j},\boldsymbol{k}\ell} = \sum_{\sigma,\tau\in S_n} \delta_i^{\ell\sigma}\delta^j_{k_\tau}\tilde{W}_g^{n,0}(|\sigma\circ\tau^{-1}|, N_c)$$

$$\mathcal{I}^{N_c+1,1}_{\boldsymbol{i}\boldsymbol{j},\boldsymbol{k}\ell} = \frac{1}{(N_c!)^2}\sum_{\alpha=1}^{N_c+1}\left(\prod_{r=i,j}\epsilon_{r_1,..,r_{\alpha-1},r_{\alpha+1},..,r_{N_c+1}}\right)\delta^{\ell_1}_{i_\alpha}\delta^{j_\alpha}_{k_1}\tilde{W}_g^{1,1}(\mathrm{id}, N_c)$$

Simplification: depending on the number of fermion hoppings, restrict $\tilde{W}_g$ **to the irreps consistent with the fermionic content**:

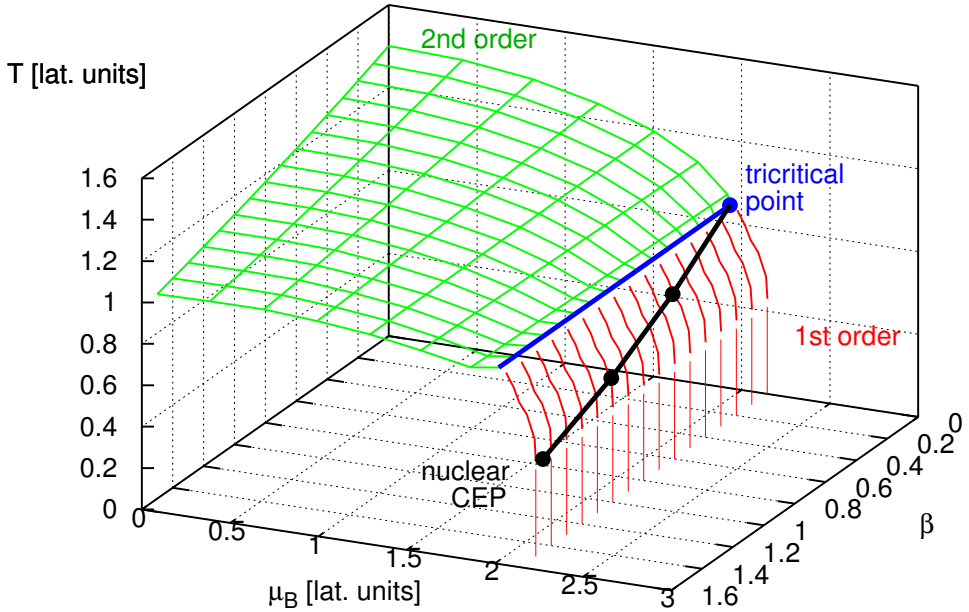
$$\tilde{W}_g^{n,q}(\rho, N_c) \to \tilde{W}_{g,\Lambda}^{n,q}(\rho, N_c) = \sum_{\substack{\lambda\in\Lambda\\ \lambda\vdash n\\ \ell(\lambda)\leq N_c}} \frac{1}{(n!)^2}\frac{f_\lambda^2\chi^\lambda(\rho)}{D_{\lambda,N_c+q}}, \qquad O(\beta):\ \Lambda = \{[1^n],[21^{n-1}]\}$$

This gives immediately:

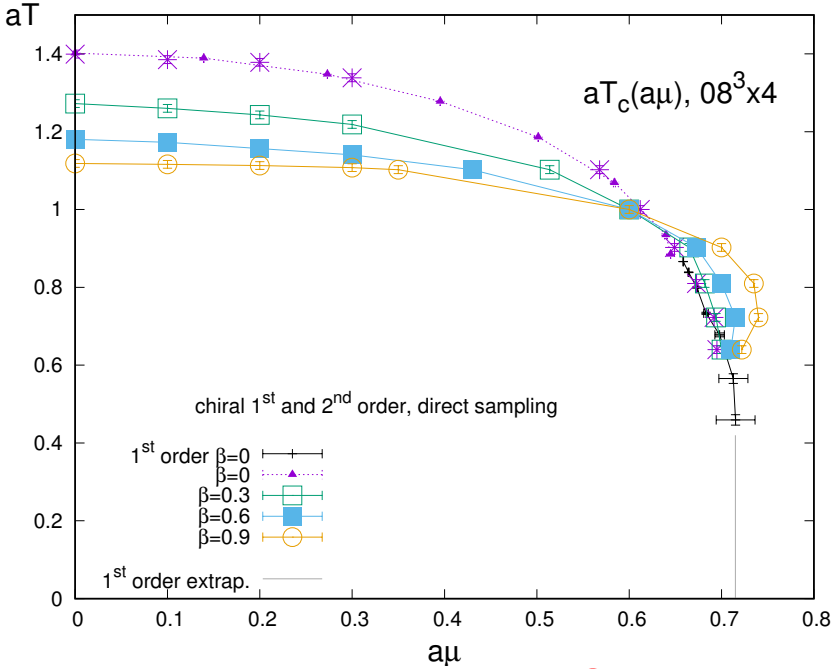
$$(J_\ell[\mathcal{M},\mathcal{M}^\dagger])^b_a = \sum_{k=1}^{N_c}\frac{(N_c-k)!}{N_c!(k-1)!}\left(M_x M_{x+\mu}\right)^{k-1}\bar{\chi}_{x,a}\chi^b_{x+\mu} + \ldots$$

$$M_x = \bar{\chi}_x\chi_x, \qquad \ell = (x,\mu)$$

$O(\beta)$ Corrections: Phase Diagram



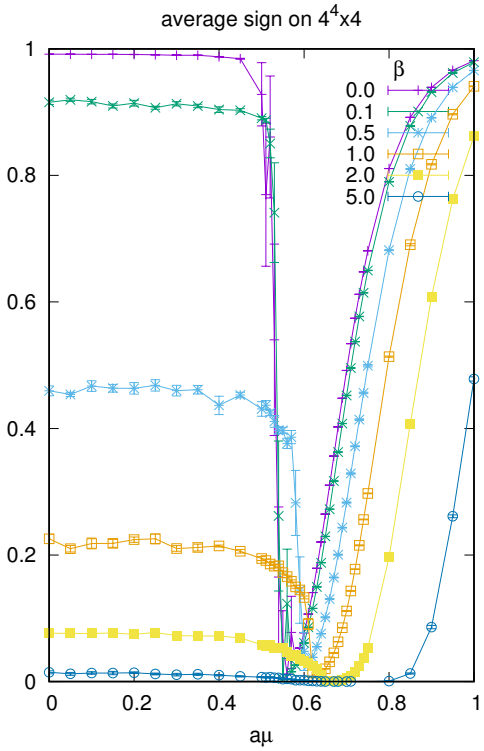
[P. De Forcrand & al., '14]

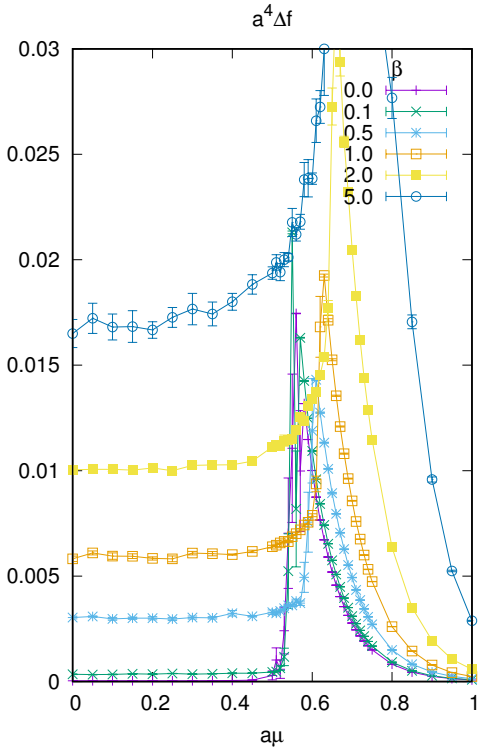


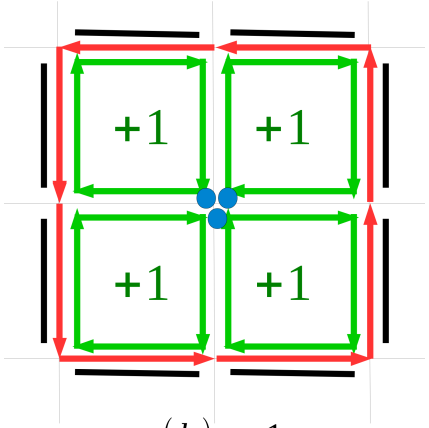
w. plaquette surfaces

- $T_c(\mu = 0)$ moves to lower values at $\beta > 0$.
- Tricritical point slightly changes with β at leading order.
- Chiral and nuclear transition **do not split** at $O(\beta)$.

$O(\beta)$ Corrections: Sign Problem







$\sigma(l_f) = -1$

winding no. $= 0$
negative quark hopings $= 4$
no. of quark loops $= -1$
$\prod_{(x,\mu)\in l_f} \eta_\mu(x) = 1$

- Complex phase goes quickly to zero for $\beta > 1$. Sign problem gets worse **at $\mu = 0$ as well**.
- Diagrammatic origin: **Frustrated monomers**, N_c-fluxes and dimers perpendicular on a plaquette surface.

As a **plaquette-induced** sign problem is present at $\mu = 0$, try to find a positive representation for pure Yang-Mills theory.

Dualization of pure Yang-Mills theory

Strong Coupling Expansion for Y-M theory

$$\mathcal{Z}_{YM} = \int_{SU(N)} [dU] e^{\frac{\beta}{2N_c} \sum_p \left[\mathrm{Tr} U_p + \mathrm{Tr} U_p^\dagger \right]}$$

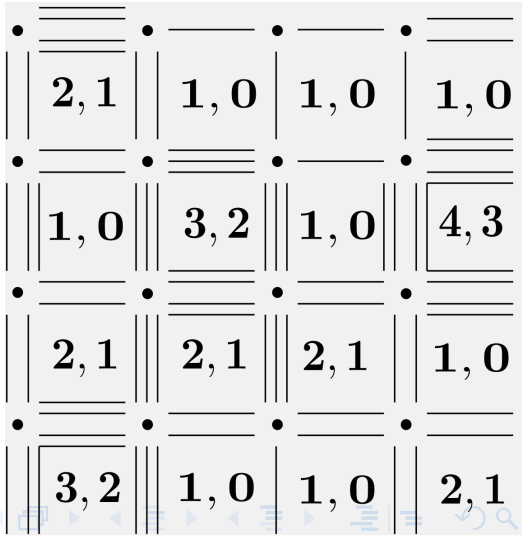
- **Taylor expand** the action in terms of plaquette(anti-plaquette) occupation numbers $\{n_p, \bar{n}_p\}$:

$$\mathcal{Z}_{YM} = \sum_{\{n_p, \bar{n}_p\}} \frac{(\beta/2N_c)^{\sum_p n_p + \bar{n}_p}}{\prod_p n_p! \bar{n}_p!} \underbrace{\prod_\ell \prod_p \int_{SU(N)} dU_\ell \left(\mathrm{Tr} U_p\right)^{n_p} \left(\mathrm{Tr} U_p^\dagger\right)^{\bar{n}_p}}_{\mathbf{W}(\{\mathbf{n_p}, \bar{\mathbf{n}}_\mathbf{p}\})}$$

- **Plaquette constraint:** For each link $\ell = (x, \mu)$:

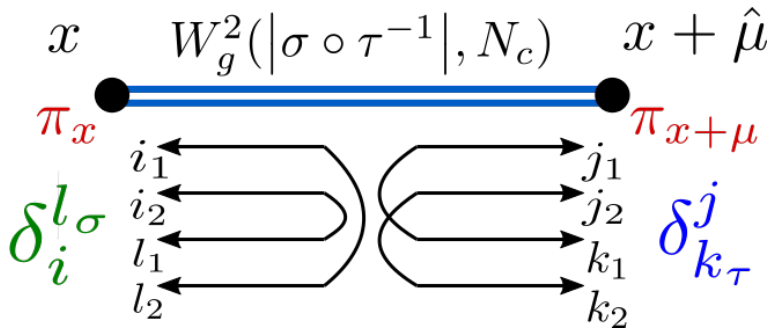
$$\sum_{\nu > \mu} \underbrace{\delta n_{x,\mu,\nu} - \delta n_{x-\nu,\mu,\nu}}_{\delta \mathbf{n_p} = \mathbf{n_p} - \bar{\mathbf{n}}_\mathbf{p}} = \begin{cases} 0 \ \mathbb{U}(\mathbb{N}) \\ 0 \ mod \ N \ \mathbb{SU}(\mathbb{N}) \end{cases}$$

$$\underbrace{d_{\ell=(x,\mu)}}_{\textbf{dimer number}} := \min \left\{ \begin{array}{c} \sum_{\nu > \mu} n_{x,\mu,\nu} + \bar{n}_{x-\nu,\mu,\nu} \\ \sum_{\nu > \mu} \bar{n}_{x,\mu,\nu} + n_{x-\nu,\mu,\nu} \end{array} \right\}$$



Dual form of the partition function: U(N) case

$$\mathcal{I}^{n,n}_{\boldsymbol{i}\boldsymbol{j},\boldsymbol{k}\ell} = \sum_{\sigma,\tau\in S_n} W_g^n(|\sigma\circ\tau^{-1}|, N_c)\delta_i^{\ell_\sigma}\delta^j_{k_\tau}$$



For $U(N)$ only the $\mathcal{I}^{a,b}$ with $a = b$ are non-zero. $W(\{n_p, \bar{n}_p\})$ can be evaluated as follows:

- Associate a pair of permutation $(\sigma_\ell, \tau_\ell) \in S_{d_\ell}$ to each **bond**.
- The **delta functions** δ^σ and δ_τ contract on each **vertex**.
- An additional permutation π_x sitting on each vertex tells us how to **re-orient the color flux**:
  - i.e. how to contract the indices between δ's associated to links that join the same vertex.

$$W(\{n_p, \bar{n}_p\}) = \sum_{\{\sigma_\ell,\tau_\ell\in S_{d_\ell}\}} \prod_\ell \underbrace{W_g^{d_\ell}(|\sigma_\ell\circ\tau_\ell^{-1}|, N_c)}_{\gtrless 0} \underbrace{\prod_x N_c^{\ell(\hat{\sigma}\circ\pi_x)}}_{\text{from delta contraction}}$$

Dual form of the partition function: U(N) case

- **Problems:** Analytic resummation too expensive. Half of the W_g's are negative. No possibility of reweighting. E.g. :

$$\tilde{W}_g^{2,0}(2, N_c) = \frac{-1}{N_c(N_c^2 - 1)}$$

- **Idea:** Express the Gauge Integrals in a different basis by introducting a new class of operators $P_\lambda^{a,b}$:

$$\mathcal{I}_{ij\,k\ell}^{n,n} = \sum_{\substack{\lambda \vdash n \\ \ell(\lambda) \leq N_c}} \frac{1}{D_{\lambda,N_c}} \cdot \left(P_\lambda^{a,b}\right)_i^\ell \left(P_\lambda^{a,b}\right)_k^j \qquad P_\lambda^{a,b} = \frac{1}{f_\lambda} \sum_{\pi \in S_n} M_\lambda^{a,b}(\pi)\delta_\pi$$

- $M_\lambda^{a,b}(\pi)$ are the matrix elements of the **irrep.** λ of S_n in the **Young-Yamanouchi** basis.
- $M_\lambda(\pi)$ is an orthogonal matrix for all $\pi \in S_n$.
- Matrix elements computed using computer algebra.

Dual form of the partition function: U(N) case

Properties of the operators $P_\lambda^{a,b}$

- Define **hermitian product** between operators in $(\mathbb{C}^{N_c})^{\otimes n}$:
  $\langle A, B\rangle := \mathrm{Tr}(A^\dagger B) \implies \langle \delta_\pi, \delta_\sigma\rangle = N_c^{\ell(\sigma\circ\pi^{-1})}$
- $P_\lambda^{a,b}$ is a complete, **orthogonal set**, with respect to $\langle\cdot\rangle$. We obtain:

$$W(\{n_p,\bar{n}_p\}) = \sum_{\substack{\{\lambda_\ell \vdash d_\ell\} \\ \ell(\lambda_\ell)\leq N_c}} \overbrace{\left[\sum_{a_\ell,b_\ell}\prod_\ell \frac{1}{D_{\lambda_\ell,N_c}}\prod_x w(x)\right]}^{W(\{n_p,\bar{n}_p\},\{\lambda_\ell\})\geq 0}$$

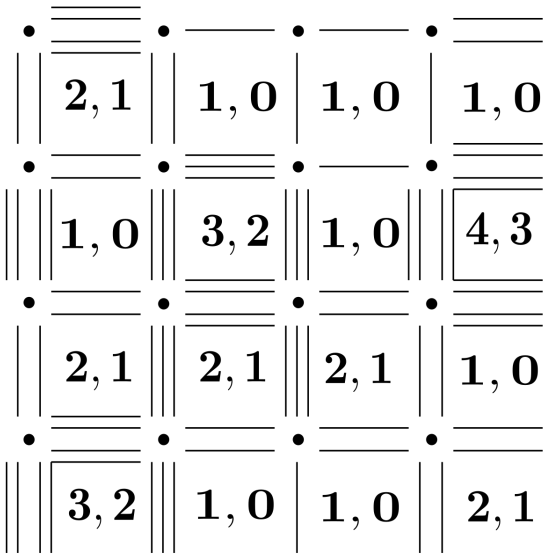
$$w(x) = \langle \otimes_{\ell\in nb(x)} P_{\lambda_\ell}^{a_\ell,b_\ell}, \delta_{\pi_x}\rangle$$

Advantages: Quantity in brackets is positive and much faster to compute $\implies$ **allows for importance sampling**. Orthogonality helps us understanding which configurations have non zero weight. Extension to $SU(N)$ easier in this orthogonal basis.

Numerical cost

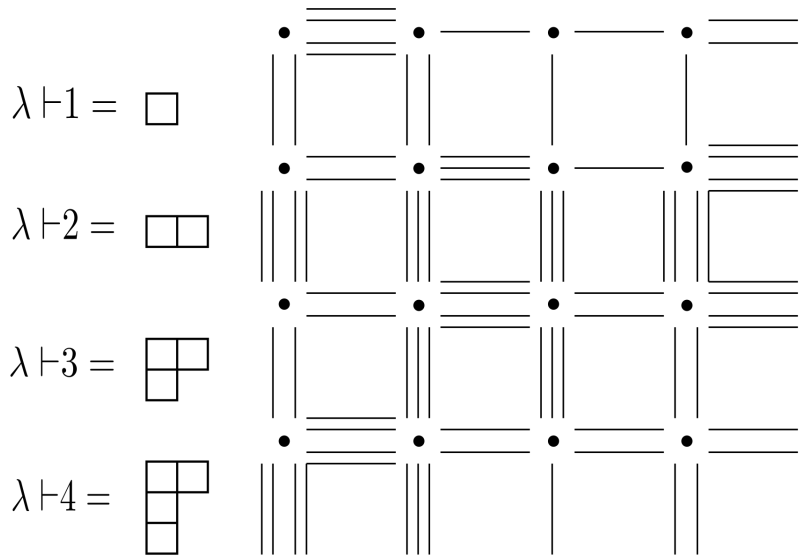
A bottleneck:

Weingarten based



operations: $\prod_\ell (d_\ell!)^2 \approx 4 \cdot 10^{36}$

Projectors based



operations: $\prod_\ell (f_{\lambda_\ell})^2 \approx 1.7 \cdot 10^{11}$

Complexity to evaluate Monte Carlo weights **still prohibitive**.

How to deal with it?

- Tabularize the weights (β-dependence **factorizes**).
- Tensor-network based methods?

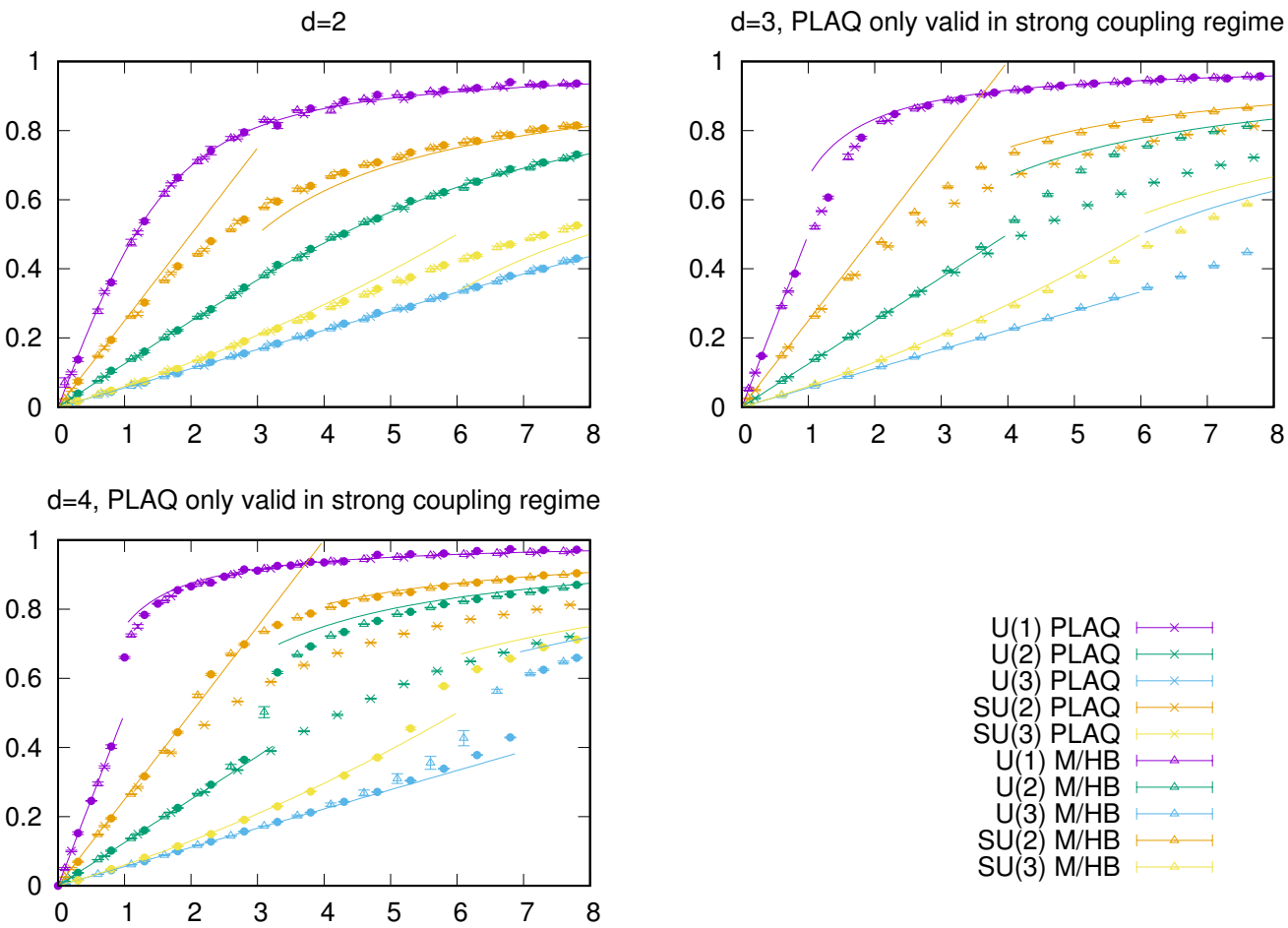
Summary

- **Results:**
  - We successfully computed all the Gauge Integrals needed to handle the plaquette contributions at $\beta > 0$.
  - We obtained a **fully dualized** partition function for *Yang-Mills* theory.
  - We checked the correctness of our approach comparing with known results.
  - By resumming a subset of weights we obtained **only positive configurations** which are labelled by integer partitions.
- **Outlook:**
  - Speedup the computation of the Monte Carlo weights.
  - Implement a Markov Chain Monte Carlo simulation for the dualized partition function.
  - Extend our approach to matter fields: scalar QCD, staggered fermions.

Backup slides

Average plaquette for pure Yang-Mills in the dual representation and comparison with standard heat bath algorithm for various dimensions:

- Weights computed using **invariants** (valid for $n_p - \bar{n}_p \bmod N_c = 0$)
- Cube updates **still missing**.



Observables in the dual representation

- Mean plaquette:

$$\left\langle \frac{\mathrm{Re}\,\mathrm{Tr}\, U_{\mu,\nu}(x)}{N_c} \right\rangle \overset{\textbf{dual}}{=} \left\langle \frac{2n_{x,\mu,\nu}}{\beta} \right\rangle$$

- Scalar glueball $J^{PC} = 0^{++}$: Extracted from temporal correlator of spatial plaquettes:

$$\begin{aligned} C(t) &= \langle \psi(t)\psi(0)\rangle - \langle \psi(t)\rangle\langle \psi(0)\rangle \\ \psi(t) &= \frac{1}{N_c}\sum_{\vec{x}}\sum_{\mu<\nu}^{\mu\neq 0} \mathrm{Re}\,\mathrm{Tr}\, U_{\mu,\nu}(\vec{x},t) \overset{\textbf{dual}}{=} \sum_{\vec{x}}\sum_{\mu<\nu}^{\mu\neq 0} \frac{n_{(\vec{x},t),\mu,\nu} + \bar{n}_{(\vec{x},t),\mu,\nu}}{\beta} \end{aligned}$$

Prospects for MC simulation

Our new degrees of freedom are $\{n_p, \bar{n}_p\}$ and integer partitions $\lambda_\ell \vdash d_\ell$.

- Different types of updates to ensure **ergodicity** without violating the **plaquette constraint**:

1) Select a plaquette p' and propose $(n_{p'}, \bar{n}_{p'}) \to (n_{p'} \pm 1, \bar{n}_{p'} \pm 1)$. Randomly choose new partitions $\lambda'_{\ell'}$ on links $\ell' \in p'$. Accept new configuration with probability:

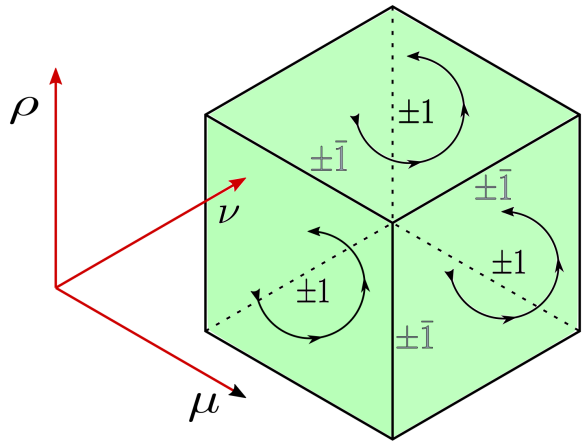
$$P_{acc} = \min\left\{1, \frac{(\beta/2N_c)^{\pm 2}}{\left[(n_{p'} \pm 1)\cdot(\bar{n}_{p'} \pm 1)\right]^{\pm 1}} \cdot \frac{W\left(\{n_p \pm \delta_{p,p'}, \bar{n}_p \pm \delta_{p,p'}\}, \{\lambda'_\ell\}\right)}{W(\{n_p, \bar{n}_p\}, \{\lambda_\ell\})}\right\}$$

2) Select a plaquette **p** and propose $n_p \to n_p \pm N_c$ or $\bar{n}_p \to \bar{n}_p \pm N_c$.

3) **At fixed** $\{n_p, \bar{n}_p\}$ select a random link ℓ' and accept $\lambda_{\ell'} \to \lambda'_{\ell'}$ with probability:

$$P_{acc} = \min\left\{1, \frac{W\left(\{n_p, \bar{n}_p\}, \{\lambda'_\ell\}\right)}{W(\{n_p, \bar{n}_p\}, \{\lambda_\ell\})}\right\}$$

4) Propose **cube updates** to change $n_p - \bar{n}_p \mod N_c$



$\mu < \nu < \rho$