Towards a Dual Representation of Lattice QCD

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Motivations

Why to use dual representations for finite density lattice QCD?
Simulations at finite $\mu_B$ 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!**

$\Rightarrow$ 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 \( \beta = \frac{2N_c}{g^2} \).

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

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

**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.

\[
Z_{sc} = \int [dU] \int d\chi \bar{\chi} e^{-(S_g + S_f)}
\]
The strong coupling partition function

- The 1-link integral can be performed analytically:

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

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

\[
Z_{SC}(m_q, \mu) = \sum_{\{k, n, \ell\}} \prod_{b=(x, \mu)} \frac{(N_c - k_b)!}{N_c! k_b!} \prod_x \frac{N_c!}{n_x!} (2am_q)^{n_x} \prod_\ell w(\ell, \mu)
\]

\[
\text{meson hoppings } M_x M_y, \quad \text{chiral cond. } \bar{\chi} \chi, \quad \text{baryon hoppings } \bar{B}_x B_y
\]

- 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 $w(\ell, \mu)$.
Advantages:

- Average complex phase $\langle e^{i\phi} \rangle_{pq} = e^{-\frac{V}{T}(f_{pq} - f)}$ close to one.  
  $\Rightarrow$ 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] $\Rightarrow$ MDP formulation.
- $\beta$ corrections to strong coupling needed to make the lattice finer. Plaquette excitations produce world sheets bounded by quark fluxes: 

\[ O(\beta) \]

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

Caveat: Dual representation does not solve, *per se*, 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 $O(\beta)$:

\[
\prod_{\ell} \int dU_\ell e^{\frac{\beta}{2N_c} \text{Tr}[U_p + U_p^\dagger]} \cdot e^{\text{Tr}[U_\ell M_\ell^\dagger + U_\ell^\dagger M_\ell]} \approx \\
\prod_{\ell} \int dU_\ell (1 + \frac{\beta}{2N_c} \text{Tr}[U_p + U_p^\dagger]) \cdot e^{\text{Tr}[U_\ell M_\ell^\dagger + U_\ell^\dagger M_\ell]}
\]

After the hopping expansion of the fermionic action:

\[
\prod_{\ell \in p} \int dU_\ell \frac{\beta}{2N_c} \text{Tr}[U_p] e^{\text{Tr}[U_\ell M_\ell^\dagger + U_\ell^\dagger M_\ell]} = \text{Tr}[\prod_{\ell \in p} J_\ell]
\]

\[
(J_\ell[M, M^\dagger])^n_m = \sum_{\kappa_\ell, \bar{\kappa}_\ell} \frac{1}{\kappa_\ell! \bar{\kappa}_\ell!} \prod_{\alpha=1}^{\kappa_\ell} (M_\ell)_{j_\alpha}^{i_\alpha} \prod_{\beta=1}^{\bar{\kappa}_\ell} (M_\ell^\dagger)_{\ell_\beta}^{k_\beta} I_{m+i, n+j, k_\ell}^{k_\ell+1, \bar{\kappa}_\ell}
\]

Gauge integral to compute
One-Link Integrals

The prototype of Gauge Integral to compute is:

\[
\mathcal{I}^{a,b}_{ij,k\ell} = \int_{SU(N_c)} dU \prod_{\alpha=1}^{a} U_{i\alpha}^{j\alpha} \prod_{\beta=1}^{b} (U^\dagger)_{k\beta}^{\ell\beta} \quad |a - b| = q \cdot N_c
\]

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

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

\[
n = \min\{a, b\} \quad (qN_c + n)! \prod_{i=0}^{N_c-1} \frac{j!}{(i + q)!} (\det K)^q \sum_{\rho \vdash n} \tilde{\mathcal{W}}^{n,q}_{g}(\rho, N_c) t_{\rho}(JK)
\]

- Baryonic contrib.
- Mesonic contrib.

\[
\tilde{\mathcal{W}}^{n,q}_{g}(\rho, N_c) = \sum_{\ell(\lambda) \leq N_c} \frac{1}{(n!)^2} \frac{f^2_{\lambda} \chi^{\lambda}(\rho)}{D_{\lambda,N_c+q}}
\]

\[
t_{\rho}(A) = \prod_{\rho_i} \text{Tr}(A^{\rho_i})
\]
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 \( \lambda \) 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 \( \rho \). Conjugacy classes of permutations can also be represented as integer partitions.

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

Conjugacy classes of permutations can also be represented as integer partitions.

\[
\ell(\lambda) = 4
\]

<table>
<thead>
<tr>
<th>\lambda</th>
<th>\lambda_1</th>
<th>\lambda_2</th>
<th>\lambda_3</th>
<th>\lambda_4</th>
</tr>
</thead>
<tbody>
<tr>
<td>9</td>
<td>4</td>
<td>2</td>
<td>2</td>
<td>1</td>
</tr>
</tbody>
</table>

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

\( \mathcal{I}^{a,b} \) 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 \(O(\beta)\):

\[
\mathcal{I}_{i,j,k}^{n,n} = \sum_{\sigma,\tau \in S_n} \delta_i^\ell \delta_j^k \tilde{\mathcal{W}}_{g}^{n,0}(|\sigma \circ \tau^{-1}|, N_c)
\]

\[
\mathcal{I}_{i,j,k}^{N_c+1,1} = \frac{1}{(N_c!)^2} \sum_{\alpha=1}^{N_c+1} \left( \prod_{r=i,j} \varepsilon_r, \ldots, r_{\alpha-1}, r_{\alpha+1}, \ldots, r_{N_c+1} \right) \delta_i^\ell \delta_j^k \tilde{\mathcal{W}}_{g}^{1,1}(\text{id}, N_c)
\]

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

\[
\tilde{\mathcal{W}}_g^{n,q}(\rho, N_c) \rightarrow \tilde{\mathcal{W}}_g^{n,q}(\rho, N_c) = \sum_{\lambda \in \Lambda} \frac{1}{(n!)^2} \frac{f_\lambda^2 \chi^\lambda(\rho)}{D_\lambda, N_c+q}
\]

\(O(\beta)\) : \(\Lambda = \{[1^n], [21^{n-1}]\}\)

This gives immediately:

\[
(J_\ell [\mathcal{M}, \mathcal{M}^\dagger])_a^b = \sum_{k=1}^{N_c} \frac{(N_c - k)!}{N_c!(k - 1)!} (M_x M_{x+\mu})^{k-1} \bar{\chi}_x a \chi_{x+\mu}^b + \ldots
\]

\(M_x = \bar{\chi}_x \chi_x, \quad \ell = (x, \mu)\)
$O(\beta)$ Corrections: Phase Diagram

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

[P. De Forcrand & al., '14]
$O(\beta)$ Corrections: Sign Problem

- 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

\[ Z_{YM} = \int_{SU(N)} [dU] e^{\frac{\beta}{2N_c} \sum_p [\text{Tr} U_p + \text{Tr} U_p^\dagger]} \]

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

\[
Z_{YM} = \sum_{\{n_p, \bar{n}_p\}} \frac{(\beta/2N_c) \sum_p n_p + \bar{n}_p}{\prod_p n_p! \bar{n}_p!} \prod_\ell \prod_p \int_{SU(N)} dU_\ell (\text{Tr} U_p)^{n_p} (\text{Tr} U_p^\dagger)^{\bar{n}_p} \]

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

\[
\sum_{\nu > \mu} \delta n_{x,\mu,\nu} - \delta n_{x-\nu,\mu,\nu} = \begin{cases} 0 & \text{U}(N) \\ 0 \mod N & \text{SU}(N) \end{cases}
\]

\[
\delta n_p = n_p - \bar{n}_p
\]

\[
d_\ell(x,\mu) := \min \left\{ \sum_{\nu > \mu} n_{x,\mu,\nu} + \bar{n}_{x-\nu,\mu,\nu}, \sum_{\nu > \mu} \bar{n}_{x,\mu,\nu} + n_{x-\nu,\mu,\nu} \right\}
\]
Dual form of the partition function: U(N) case

\[ I_{i,j,k}^{n,n} = \sum_{\sigma,\tau \in S_n} W^n_g(\lvert \sigma \circ \tau^{-1} \rvert, N_c) \delta_{i}^{\ell} \delta_{k}^{\tau} \]

For U(N) only the \( I^{a,b} \) 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 \( \delta_{\sigma} \) and \( \delta_{\tau} \) contract on each vertex.
- An additional permutation \( \pi_{x} \) sitting on each vertex tells us how to re-orient the color flux:
  - i.e. how to contract the indices between \( \delta \)'s associated to links that join the same vertex.

\[
W(\{n_p, \bar{n}_p\}) = \sum_{\{\sigma_{\ell}, \tau_{\ell} \in S_{d_{\ell}}\}} \prod_{\ell} W^d_{g}(\lvert \sigma_{\ell} \circ \tau_{\ell}^{-1} \rvert, N_c) \prod_{x} N_{c}^{\ell}(\hat{\sigma} \circ \pi_{x}) \]

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.:

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

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

$$\mathcal{I}^{n,n}_{i,j,k,l} = \sum_{\lambda \vdash n, \ell(\lambda) \leq N_c} \frac{1}{D_{\lambda,N_c}} \cdot (P^{a,b}_\lambda)^{i}_{j} (P^{a,b}_\lambda)^{j}_{k} \quad P^{a,b}_\lambda = \frac{1}{f_{\lambda}} \sum_{\pi \in S_n} M^{a,b}_\lambda(\pi) \delta_\pi$$

- $M^{a,b}_\lambda(\pi)$ are the matrix elements of the **irrep.** $\lambda$ 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.
Properties of the operators $P^a, b_\lambda$

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

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

\[
w(x) = \langle \bigotimes_{\ell \in nb(x)} P_{\lambda_\ell}^{a_\ell, b_\ell}, \delta_{\pi x} \rangle
\]

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

**A bottleneck:**

<table>
<thead>
<tr>
<th>Weingarten based</th>
<th>Projectors based</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2, 1)</td>
<td>(\lambda \downarrow 1) =</td>
</tr>
<tr>
<td>(1, 0)</td>
<td>(\lambda \downarrow 2) =</td>
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</tr>
</tbody>
</table>

| \(\prod_{\ell} (d_{\ell}!)^2 \approx 4 \cdot 10^{36}\) | \(\prod_{\ell} (f_{\lambda \ell})^2 \approx 1.7 \cdot 10^{11}\) |

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

**How to deal with it?**

- Tabularize the weights (\(\beta\)-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 $n_p - \bar{n}_p \mod N_c = 0$)
- Cube updates **still missing**.
Observables in the dual representation

Mean plaquette:

\[
\left\langle \frac{\text{Re Tr } U_{\mu,\nu}(x)}{N_c} \right\rangle_{\text{dual}} = \left\langle \frac{2n_{x,\mu,\nu}}{\beta} \right\rangle
\]

Scalar glueball \( J^{PC} = 0^{++} \): Extracted from temporal correlator of spatial plaquettes:

\[
C(t) = \langle \psi(t)\psi(0) \rangle - \langle \psi(t) \rangle \langle \psi(0) \rangle
\]

\[
\psi(t) = \frac{1}{N_c} \sum_{\vec{x}} \sum_{\mu \neq 0} \sum_{\mu < \nu} \text{Re Tr } U_{\mu,\nu}(\vec{x}, t)_{\text{dual}} = \sum_{\vec{x}} \sum_{\mu \neq 0} \frac{n_{\vec{x},t},\mu,\nu + \bar{n}_{\vec{x},t},\mu,\nu}{\beta}
\]
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 \((n_{p'}, \bar{n}_{p'}) \rightarrow (n_{p'} \pm 1, \bar{n}_{p'} \pm 1)\). Randomly choose new partitions \( \lambda'_{\ell'} \) on links \( \ell' \in p' \). Accept new configuration with probability:

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

2. Select a plaquette \( p \) and propose \( n_p \rightarrow n_p \pm N_c \) or \( \bar{n}_p \rightarrow \bar{n}_p \pm N_c \).

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

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

4. Propose **cube updates** to change \( n_p - \bar{n}_p \mod N_i \).