Hamiltonian Lattice QCD from Strong Coupling Expansion

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with Pratitee Pattanaik

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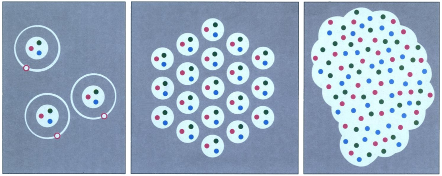


UNIVERSITÄT BIELEFELD
Faculty of Physics

CRC–TR 211
Strong-interaction matter under extreme conditions

Outline

Context:

- **Quantum Hamiltonian LQCD:** has been established for $N_\mathrm{f} = 1$ and the strong coupling limit only
- allows to apply **Quantum Monte Carlo algorithms** for finite μ_B

[Klegrewe, U. PRD 102 (2020)]

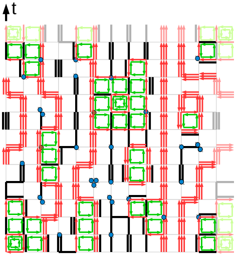
Aim:

Determine the phase diagram for
both finite baryon and isospin chemical potential

Content of the talk:

1. Quick overview of the $N_\mathrm{f} = 1$ Hamiltonian
2. Evaluation of the $N_\mathrm{f} = 2, 3$ Hamiltonian
3. Discussion of the gauge corrections $\mathcal{O}(\beta)$ to Hamiltonian

- **Dual representation**: color singlets from integrating out gauge fields $U_\mu(x)$
  - unrooted staggered fermions, standard Wilson gauge action
  - at $\beta = 0$: link states are **mesons** and **baryons** [Rossi, Wolff, NPB 248 (1984)]
  - at $\beta > 0$: color singlets may include gluon contributions [Gagliardi, U, PRD 101 (2020)]



2-dim. example of configuration in terms of dual variables

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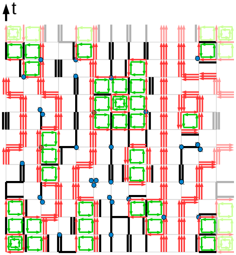
  - at $\beta > 0$: color singlets may include gluon contributions [Gagliardi, U, PRD 101 (2020)]
- Sign problem in regime $\beta = \frac{6}{g^2} \lesssim 1$ **mild enough** to study full phase diagram:
  - baryons are heavy: $\Delta f \simeq 10^{-5}$
  - in continuous time limit $N_t \to \infty$: **baryons become static**

    $\Rightarrow$ finite density sign problem absent!



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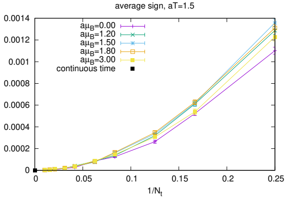

average sign vanishes for $N_t \to \infty$ $(a_t \to 0)$

Quantum Hamiltonian is derived from dual representation via continuous time limit!

Euclidean Continuous Time Limit

Introduce **bare anisotropy** γ in Dirac couplings such that $\xi = \frac{a_s}{a_t} \neq 1$:

$$Z_F(m_q, \mu, \gamma) = \sum_{\{k,n,\ell\}} \prod_{b=(x,\mu)} \frac{(N_c - k_b)!}{N_c! k_b!} \gamma^{2 k_b \delta_{\mu 0}} \prod_x \frac{N_c!}{n_x!} (2 a m_q)^{n_x} \prod_\ell w(\ell, \mu)$$

- Non-perturbative result: $\xi(\gamma) \approx \kappa \gamma^2 + \frac{\gamma^2}{1+\lambda\gamma^4}, \quad \kappa = 0.781(1)$

  [de Forcrand, Vairinhos, U., PRD 97 (2018)]

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Define the **continuous Euclidean time limit** (CT-limit):

$$\boxed{N_t \to \infty, \quad \xi, \gamma \to \infty, \quad aT = \frac{\xi(\gamma)}{N_t} \simeq \kappa \mathcal{T}(\gamma, Nt), \quad \mathcal{T} = \frac{\gamma^2}{N_t} \quad \text{fixed}}$$

- **only one parameter** $\mathcal{T}$ setting the temperature

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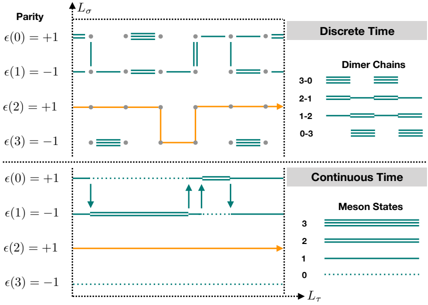
Main **advantages** of CT-limit:

- no need to perform the continuum extrapolation $a_t \to 0$ ($N_t \to \infty$)
- determine phase boundary unambiguously and more precisely, with a faster algorithm (QMC)

From Dimers to Meson Occupation Numbers $(N_\mathrm{f} = 1)$

Correspondence between discrete and continuous time:

- **alternating dimer chains** (top) and **meson occupation numbers** in continuous time (bottom):
- multiple spatial dimers become **resolved in single spatial dimers** and can be oriented consistently due to even-odd ordering



- definition of **meson occupation number** $\mathfrak{m}(x)$

$$k_0(x) \mapsto \mathfrak{m}(x) = \epsilon(x)\left(k_0(x) - \frac{N_\mathrm{c}}{2}\right) + \frac{N_\mathrm{c}}{2}, \quad \mathfrak{m}(x) \in \{0, 1, \ldots N_\mathrm{c}\}$$

  with $\epsilon(x) = \pm 1$ the parity of a site

- **conservation law:** for dimer connecting $\langle x, y \rangle$

$$\mathfrak{m}_x \mapsto \mathfrak{m}_x \pm 1 \quad \Leftrightarrow \quad \mathfrak{m}_y \mapsto \mathfrak{m}_y \mp 1$$

Hamiltonian Formulation: Creation and Annihilation Operators

Derive Hamiltonian via **diagrammatic expansion** of $Z_{CT} = \lim_{\gamma, N_t \to \infty} Z_{N_t}(\gamma)$

- express the partition function as series in inverse temperature $\frac{1}{\mathcal{T}} = \frac{N_t}{\gamma^2}$:

$$Z_{\mathrm{CT}}(\mathcal{T}, \mu_{\mathcal{B}}) = \mathrm{Tr}_{\mathfrak{h}} \left[e^{(\hat{\mathcal{H}} + \hat{\mathcal{N}} \mu_{\mathcal{B}})/\mathcal{T}} \right], \; \hat{\mathcal{H}}_I = \frac{1}{2} \sum_{\langle \vec{x}, \vec{y} \rangle} \left(\hat{J}^+_{\vec{x}} \hat{J}^-_{\vec{x}} + \hat{J}^-_{\vec{x}} \hat{J}^+_{\vec{x}} \right), \; \hat{\mathcal{N}} = \sum_{\vec{x}} \hat{\omega}_x$$

- the **creation** $\hat{J}^+$ and **annihilation operators** $\hat{J}^- = (\hat{J}^+)^T$ contain the matrix elements $\langle \mathfrak{m}_1 | 1 | \mathfrak{m}_2 \rangle$ with $\hat{v}_{\mathsf{L}} = \langle 0|1|2 \rangle = 1$, $\hat{v}_{\mathsf{T}} = \langle 1|1|1 \rangle = \frac{\sqrt{3}}{4}$:

$$\hat{J}^+ = \left(\begin{array}{cccc|cc} 0 & 0 & 0 & 0 & & \\ \hat{v}_{\mathsf{L}} & 0 & 0 & 0 & & \\ 0 & \hat{v}_{\mathsf{T}} & 0 & 0 & & \\ 0 & 0 & \hat{v}_{\mathsf{L}} & 0 & & \\ \hline & & & & 0 & 0 \\ & & & & 0 & 0 \end{array} \right), \quad \hat{\omega} = \left(\begin{array}{cccc|cc} 0 & 0 & 0 & 0 & & \\ 0 & 0 & 0 & 0 & & \\ 0 & 0 & 0 & 0 & & \\ 0 & 0 & 0 & 0 & & \\ \hline & & & & 1 & 0 \\ & & & & 0 & -1 \end{array} \right)$$

- **local Hilbert space** per site: $|\mathfrak{h}\rangle \in \mathbb{H}_{\mathfrak{h}} = [0, \pi, 2\pi, 3\pi; B^+, B^-]$
- block-diagonal structure due to commutation relation $[\hat{\mathcal{H}}, \hat{\mathcal{N}}] = 0$

Interpretation:

- Pauli saturation holds on the level of the quarks and pions have a fermionic substructure, $|\mathfrak{m}\rangle$ **bounded from above**
  $\Rightarrow$ **particle-hole symmetry**, leading to **"spin" algebra**:

$$\hat{J}_1 = \frac{\sqrt{N_\mathrm{c}}}{2}\left(\hat{J}^+ + \hat{J}^-\right), \quad \hat{J}_2 = \frac{\sqrt{N_\mathrm{c}}}{2i}\left(\hat{J}^+ - \hat{J}^-\right),$$

$$\hat{J}_3 = i[J_1, J_2] = \frac{N_\mathrm{c}}{2}[\hat{J}^+, \hat{J}^-], \quad \hat{J}^2 = \frac{N_\mathrm{c}(N_\mathrm{c}+2)}{4}$$

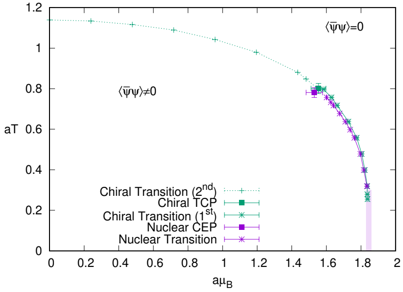
- the "spin"-representation is $d = N_\mathrm{c}+1$**-dimensional**, with $S = N_\mathrm{c}/2$.

$$\mathfrak{m} \mapsto \mathfrak{s} = \mathfrak{m} - \frac{N_\mathrm{c}}{2}: \qquad \hat{J}_3\left|\frac{N_\mathrm{c}}{2}, \mathfrak{s}\right\rangle = \mathfrak{s}\left|\frac{N_\mathrm{c}}{2}, \mathfrak{s}\right\rangle,$$

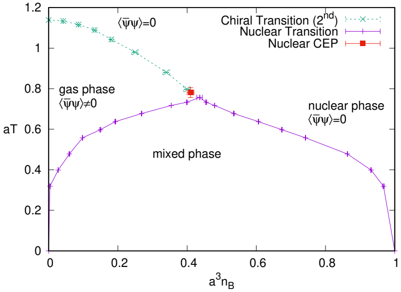
$$\hat{J}^2\left|\frac{N_\mathrm{c}}{2}\mathfrak{s}\right\rangle = \frac{N_\mathrm{c}\left(N_\mathrm{c}+2\right)}{4}\left|\frac{N_\mathrm{c}}{2}, \mathfrak{s}\right\rangle, \qquad [\hat{J}^2, \hat{J}_3] = 0.$$

From **Quantum Monte Carlo** / Density of States Method:

- obtain baryonic observables and phase diagrams to high precision



Grand-canonical phase diagram



Canonical phase diagram

[Klegrewe, U. PRD 102 (2020)]

Static Limit: Nf=2,3

Local Hilbert space $\mathbb{H}_{\mathfrak{h}}$ via canonical sectors $B \in [-N_{\rm f}, -N_{\rm f}+1, \ldots, N_{\rm f}]$:

- whereas $\mathbb{H}_{\mathfrak{h}}$ is $d = [1, (N_{\rm c}+1), 1]$-dimensional for $N_{\rm f} = 1$, it quickly grows with the number flavors
- general formula for static partition sum: [U., Lattice 2014]:

$$Z_{\rm stat}(N_{\rm c}, N_{\rm f}) \sum_{B=-Nf}^{N_{\rm f}} \prod_{a=0}^{N_{\rm c}} \frac{a!(2N_{\rm f}+a)!}{(N_{\rm f}+a+B)!(Nf+a-B)!} e^{B\mu_B/T}$$

- coefficient encodes number of **hadronic states** $\mathfrak{h}$, for gauge group $\mathrm{SU}(3)$:
  - $N_{\rm f} = 2$: $d = [1, 20, 50, 20, 1] = 92$
  - $N_{\rm f} = 3$: $d = [1, 56, 490, 980, 490, 56, 1] = 2074$

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No general formula known for isospin sectors, required for $\mu_I \neq 0$!
Individual states $\mathfrak{h}$ also required for constructing $\hat{J}^{\pm}$!

Link integration for $N_\mathrm{f} > 1$

Every state of the local Hilbert space can be described by a **set of charges**:

- $B \in \{-N_\mathrm{f}, \ldots N_\mathrm{f}\},\ I \in \{-N_\mathrm{c}, \ldots N_\mathrm{c}\},\ U, D \in \{0, \ldots N_\mathrm{c}\}$ for $N_\mathrm{f} = 2$
- $K_1, K_2 \in \{-N_\mathrm{c}, \ldots N_\mathrm{c}\},\ S \in \{0, \ldots N_\mathrm{c}\}$ additionally for $N_\mathrm{f} = 3$

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Invariant integration:

- starting point: $\mathcal{J}(\mathcal{M}, \mathcal{M}^\dagger) = \int_{\mathrm{SU}(3)} dU e^{\mathrm{Tr}[U\mathcal{M}^\dagger + U^\dagger \mathcal{M}]} = f(X, Y, Z, \Delta)$

  [Eriksson *et al.*, J. Math. Phys. 22 (1981)]
- need to rewrite basis X, Y, Z, Δ in basis X_i, D suitable for the charges
- some combinatorial tricks required, final result for $\mathrm{SU}(3)$

$$\mathcal{J}(\mathcal{M}, \mathcal{M}^\dagger) = \sum_{B=-N_\mathrm{f}}^{N_\mathrm{f}} \sum_{n_1, n_2, n_3} C_{B, n_1, n_2, n_3} \prod_{k=1}^{3} \frac{X_i^{n_k}}{n_k!} \frac{D^B}{|B|!}, \quad D = \begin{cases} \det \mathcal{M} & B > 0 \\ 1 & B = 0 \\ \det \mathcal{M}^\dagger & B < 0 \end{cases}$$

$$C_{B, n_1, n_2, n_3} = 2 \frac{\binom{n_1 + 2n_2 + 4n_3 + 2|B| + 2}{n_3 + |B|} |B|!}{(n_1 + 2n_2 + 3n_3 + 2|B| + 2)!(n_2 + 2n_3 + |B| + 1)!}$$

Link integration for $N_\mathrm{f} > 1$

Invariants in terms of nearest neighbors $(M_x M_y)^n = (-1)^{n+1}(\mathcal{M}\mathcal{M}^\dagger)^n$:

$$X_1 = \mathrm{Tr}[M_x M_y]$$

$$X_2 = X_1^2 - D_2, \qquad D_2 = \det_2[M_x M_y]$$

$$X_3 = X_1^3 - 2X_1 D_2 + D_3, \quad D_3 = \det_3[M_x M_y] \qquad (D_3 = 0 \quad \text{for} \quad N_\mathrm{f} = 2)$$

Static limit (1-dim QCD):

- proven that all states $\mathfrak{h} \in \mathbb{H}_\mathfrak{h}$ for $N_\mathrm{f} = 2, 3$ contribute with a weight 1, although some link weights are negative!
- for $N_\mathrm{f} = 2$:

$$\mathcal{Z}\left(\frac{\mu_B}{T}, \frac{\mu_I}{T}\right) = 2\cosh\frac{3\mu_I}{T} + 8\cosh\frac{2\mu_I}{T} + 20\cosh\frac{\mu_I}{T} + 20 + 2\cosh\frac{\mu_B}{T}\left(8\cosh\frac{\frac{3}{2}\mu_I}{T} + 12\cosh\frac{\frac{1}{2}\mu_I}{T}\right) + 2\cosh\frac{2\mu_B}{T}$$

- Similar result involving also μ_S for $N_\mathrm{f} = 3$ (lengthy!)

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- Similar result involving also μ_S for $N_\mathrm{f} = 3$ (lengthy!)

Ready to go beyond static limit!

Interaction Hamiltonian and Matrix Elements

- due to simplifications in limit $\gamma, N_t \to \infty$, also for $N_\mathrm{f} > 1$ **only single mesons are interchanged** between nearest neighbors
- the interaction Hamiltonian has ${N_\mathrm{f}}^2$ contributions, one for each meson:

$$\hat{\mathcal{H}}_I = \frac{1}{2} \sum_{\langle \vec{x},\vec{y} \rangle} \sum_{Q_i} \left(\hat{J}^+_{Q_i,\vec{x}} \hat{J}^-_{Q_i,\vec{y}} + \hat{J}^-_{Q_i,\vec{x}} \hat{J}^+_{Q_i,\vec{y}} \right)$$

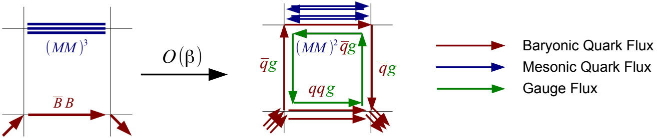
  - for $N_\mathrm{f} = 2$: $Q_i \in \{\pi^+, \pi^-, \pi_U, \pi_D\}$
  - for $N_\mathrm{f} = 3$: $Q_i \in \{\pi^+, \pi^-, K^+, K^-, K_0, \bar{K}_0, \pi_U, \pi_D, \pi_S\}$
- for the transition $\mathfrak{h}_1 \mapsto \mathfrak{h}_2$, the **matrix elements** $\left\langle \mathfrak{h}_1 | Q_i | \mathfrak{h}_2 \right\rangle$ of $\hat{J}^\pm_{Q_i}$ are determined from Grassmann integration
- only those matrix elements are non-zero which are consistent with current conservation all Q_i
- example: $\left\langle \pi_D | \pi_U | \mathfrak{m}_0^4 \right\rangle = \frac{\sqrt{5}}{6}$ with $\mathfrak{m}_0^2 = \pi^+\pi^- = \pi_U \pi_D$

- QCD Partition function via **strong coupling expansion in β:**

$$Z_{QCD} = \int d\psi d\bar{\psi} dU e^{S_G + S_F} = \int d\psi d\bar{\psi} Z_F \left\langle e^{S_G} \right\rangle_{Z_F}$$

$$\left\langle e^{S_G} \right\rangle_{Z_F} \simeq 1 + \langle S_G \rangle_{Z_F} + \mathcal{O}(\beta^2) = 1 + \frac{\beta}{2N_c} \sum_P \left\langle \mathrm{tr}[U_P + U_P^\dagger] \right\rangle_{Z_F} + \mathcal{O}(\beta^2)$$

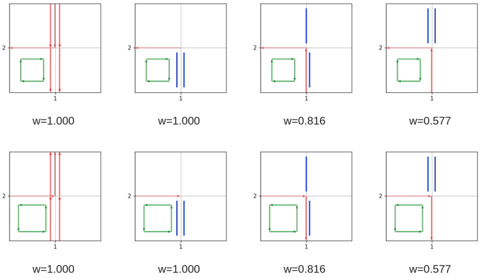
$\rightarrow$ **additional color singlet link states** due to plaquettes



- for discrete time lattices, the dual formulation has been extended beyond $\mathcal{O}(\beta)$ in terms of a **tensor network** [Gagliardi, U, PRD 101 (2020)]

Gauge contributions to the Hamiltonian $(N_f = 1)$

- on anisotropic lattices, the anisotropy $\xi = \frac{a_s}{a_t}$ is a function of two bare anisotropies γ_F and $\gamma_G = \sqrt{\frac{\beta_t}{\beta_s}}$
- in the continuous time limit $a_t \to 0$ $(\xi \to \infty)$ and for small β, spatial plaquettes are suppressed over temporal plaquettes by $(\gamma_G \gamma_F)^{-2}$
  $\Rightarrow$ only consider **temporal plaquettes:**



- temporal plaquettes are of same order as pion exchange, but also allows to **couple baryons!** ($\hat{J}^{\pm}$ still block-diagonal)

Conclusions

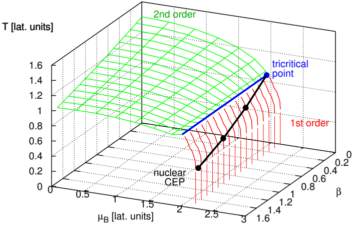
Results:

- Hamiltonian formulation also completely **sign problem-free** for $N_\mathrm{f} > 1$ (not the case for discrete N_t!)
- Matrix elements for the **creation and annihilation operators** $\hat{J}^{\pm}$ have now been determined for $N_\mathrm{f} = 2, 3$
- **Gauge corrections** of $\mathcal{O}(\beta)$ have been incorporated to Quantum Hamiltonian for $N_\mathrm{f} = 1$

Goals:

- Quantum Monte Carlo simulations for $N_\mathrm{f} > 1$
- Determine the phase diagram in the T, μ_B, μ_I-space.
- Measure nuclear potential to study pion exchange
- Include gauge corrections also for $N_\mathrm{f} > 1$

Phase Diagram in the Strong Coupling Regime: [Langelage *et al.* PRL **113** (2014)]



obtained via reweighting in β

- has a chiral and nuclear transition
- important question: what happens to the chiral (tri)-critical point?

One of several **possible scenarios** for the extension to the continuum:

- back plane: strong coupling phase diagram ($\beta = 0$, a large), $N_f = 1$
- front plane: continuum phase diagram ($\beta = \infty$, $a = 0$), $N_f = 4$ (no rooting)