Towards Quantum Monte Carlo Simulations at non-zero Baryon and Isospin Density in the Strong Coupling Regime

Wolfgang Unger, Pratitee Pattanaik, Bielefeld University

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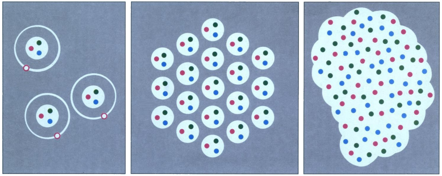


UNIVERSITÄT BIELEFELD

Faculty of Physics

CRC-TR 211

Strong-interaction matter under extreme conditions

LATTICE 2022

AUGUST 8TH–13TH BONN GERMANY

Context:

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

[Klegrewe, U. PRD 102 (2020)]

Aim:

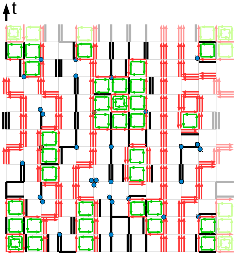
$N_\mathrm{f} = 2$: Determine the phase diagram for
both finite baryon and isospin chemical potential

Content of the talk:

1. The Hamiltonian approach to Lattice QCD
2. Expectations from Meanfield Theory and HMC for $N_\mathrm{f} = 2$
3. Setup of the $N_\mathrm{f} = 2$ Quantum Monte Carlo Simulation
4. Preliminary results at finite μ_B, μ_I

Lattice QCD in a Dual Formulation

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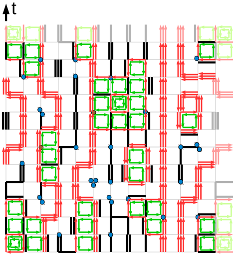
  - at $\beta > 0$: color singlets may include gluon contributions [Gagliardi, U, PRD 101 (2020)]
- Sign problem in regime $\beta = \frac{6}{g^2} \lesssim 1$ **mild enough** to study full phase diagram:
  - baryons are heavy: $\Delta f \simeq 10^{-5}$
  - in continuous time limit $N_t \to \infty$: **baryons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

    $\Rightarrow$ finite density sign problem absent!

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



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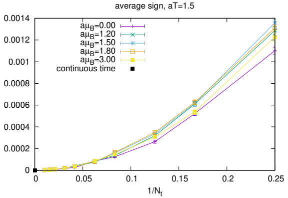

average sign vanishes for $N_t \to \infty$ $(a_t \to 0)$

Euclidean Continuous Time Limit

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

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

- 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):

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

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

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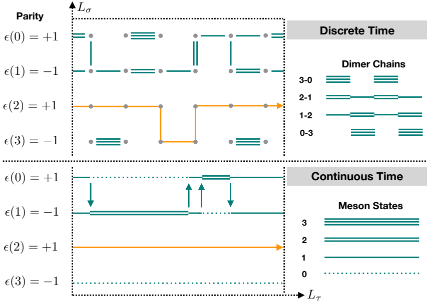
Main **advantages** of CT-limit:

- 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)

Correspondence between discrete and continuous time:

- alternating dimer chains (top) and **meson occupation numbers** $\mathfrak{m}$ (bottom):
- multiple spatial dimers become **resolved in single spatial dimers**, oriented consistently due to even-odd ordering



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

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

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 $\frac{1}{\mathcal{T}} = \frac{N_t}{\gamma^2}$:

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

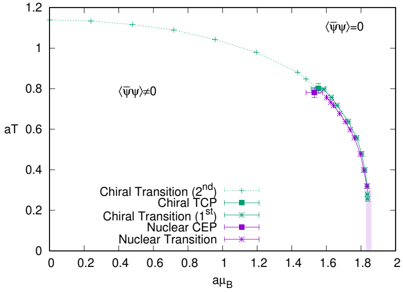
- the **creation** $\hat{J}^+$ and **annihilation operators** $\hat{J}^- = (\hat{J}^+)^T$ contain the matrix elements $\langle \mathfrak{m}_1 | 1 | \mathfrak{m}_2 \rangle$ with $\hat{v}_{\mathsf{L}} = \langle 0|1|2 \rangle = 1$, $\hat{v}_{\mathsf{T}} = \langle 1|1|1 \rangle = \frac{\sqrt{3}}{4}$:

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

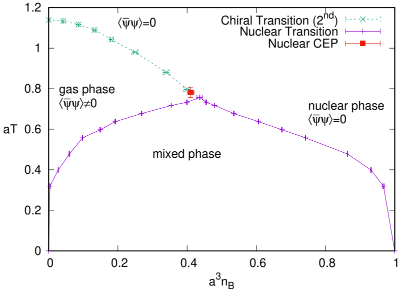
- **local Hilbert space** per site: $|\mathfrak{h}\rangle \in \mathbb{H}_{\mathfrak{h}} = [0, \pi, 2\pi, 3\pi; B^+, B^-]$
- block-diagonal structure due to commutation relation $[\hat{\mathcal{H}}, \hat{\mathcal{N}}] = 0$

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

- obtain baryonic observables and phase diagrams to high precision



Grand-canonical phase diagram

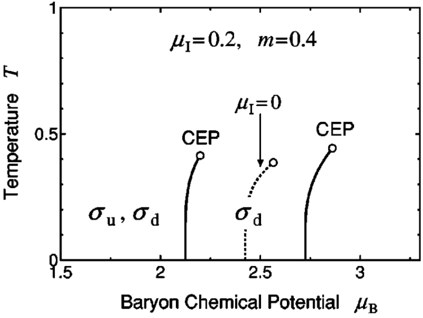


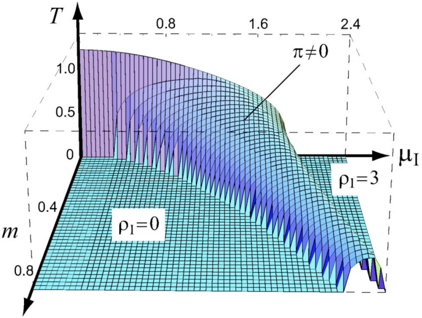
Canonical phase diagram

[Klegrewe, U. PRD 102 (2020)]

Expectations from Mean Field Theory at Strong Coupling (Nf=2)

- mean field results for staggered fermions in $1/d$ expansion
- at non-zero isospin density: two CEP (first σ_u vanishes, then σ_d)
- pion condensation vanishes again at larger isospin density (Pauli saturation)

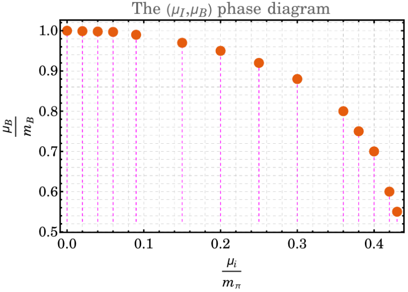




[Nishida, PRD **69 (2004)]**

Expectations from Mean Field for 3-dim Effective Theory (Nf=2)

- mean field based on Polyakov loop effective theory (Wilson fermions via hopping parameter expansion)



[from Master thesis of Amine Chabane (2022)]

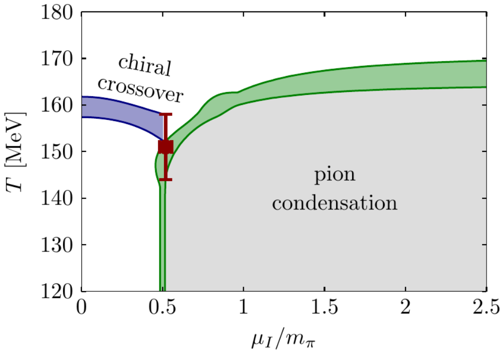
- see next talk by **Amine Chabane** "Towards the phase diagram of cold and dense heavy QCD", Mon. 5:30
  and talk by **Christoph Konrad** "Mean-field approximation of effective theories of lattice QCD", Fri. 6pm

Expectations from HMC (Nf=2+1)

QCD phase diagram at non-zero isospin chemical potential:

[Brandt et al., Confinement 2018 (260)]

- in continuum limit
- at physical quark masses



- see talk by **Bastian Brandt** "Equation of state and Taylor expansions at nonzero isospin chemical potential", Thu. 9am

Quantum Hamiltonian for $N_\mathrm{f} = 2$: Derivation

Dual representation for $N_\mathrm{f} = 2$ (not sign problem-free for finite N_t)
but sign-problem free in continuous time limit $N_t \to \infty$: [U., Lattice 2021]

- first: link integration for $N_\mathrm{f} > 1$:

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

- then: Grassmann integration for $N_\mathrm{f} > 1$
- due to continuous time limit, also for $N_\mathrm{f} > 1$,
  only single mesons are interchanged between nearest neighbors

Quantum Hamiltonian for $N_\mathrm{f} = 2$: Final Expression

The Hamiltonian has ${N_\mathrm{f}}^2$ contributions, one for each pseudoscalar meson:

- partition function:

$$Z_\mathrm{CT}(\mathcal{T}, \mu_\mathcal{B}, \mu_\mathcal{I}) = \mathrm{Tr}_\mathfrak{h}\left[e^{(\hat{\mathcal{H}}+\hat{\mathcal{N}}_B\mu_\mathcal{B}+\hat{\mathcal{N}}_I\mu_\mathcal{I})/\mathcal{T}}\right] \qquad \mathfrak{h} \in \mathbb{H}_\mathfrak{h}$$

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

- for the transition $\mathfrak{h}_1 \mapsto \mathfrak{h}_2$, the **matrix elements** $\langle\mathfrak{h}_1|Q_i|\mathfrak{h}_2\rangle$ of $\hat{J}^\pm_{Q_i}$ are determined from Grassmann integration and diagonalization
- only those matrix elements are non-zero which are consistent with current conservation of all Q_i, **and turn out to be positive!**

Local Hilbert space $\mathbb{H}_\mathfrak{h}$:

- multiplicities in basis B, I and meson occupation number m

B	I	$\mathfrak{m}=0$	$\mathfrak{m}=1$	$\mathfrak{m}=2$	$\mathfrak{m}=3$	$\mathfrak{m}=4$	$\mathfrak{m}=5$	$\mathfrak{m}=6$	Σ
-2	0	1							1
-2	Σ	1	0	0	0	0	0	0	1
-1	$-\frac{3}{2}$	1	1	1	1				4
-1	$-\frac{1}{2}$	1	2	2	1				6
-1	$+\frac{1}{2}$	1	2	2	1				6
-1	$+\frac{3}{2}$	1	1	1	1				4
-1	Σ	4	6	6	4	0	0	0	20
0	-3				1				1
0	-2			1	2	1			4
0	-1		1	2	4	2	1		10
0	0	1	2	4	6	4	2	1	20
0	-1		1	2	4	2	1		10
0	-2			1	2	1			4
0	-3				1				1
0	Σ	1	4	10	20	10	4	1	50
1	$-\frac{3}{2}$	1	1	1	1				4
1	$-\frac{3}{2}$	1	2	2	1				6
1	$+\frac{3}{2}$	1	2	2	1				6
1	$+\frac{3}{2}$	1	1	1	1				4
1	Σ	4	6	6	4	0	0	0	20
2	0	1							1
2	Σ	1	0	0	0	0	0	0	1
Σ		11	16	22	28	10	4	1	92

Hadronic states distinguished on the quark level

- state multiplicities: given B, I, m, states with same quark content have to be identified, e.g.

$$\pi_+\pi_- = \pi_U\pi_D, \qquad B_{uuu}\pi_D = B_{uud}\pi_-, \qquad B_{uuu}B_{ddd} = B_{uud}B_{udd}$$

- quark content not sufficient, some states have twofold degeneracy:

	B	I	m	quark state $\bar{u}u\bar{d}d$
36	0	0	0	0 0 0 0 (0)
37	0	0	1	0 0 1 1 (0)
38	0	0	1	1 1 0 0 (0)
39	0	0	2	0 0 2 2 (0)
40	0	0	2	1 1 1 1 (0)
41	0	0	2	1 1 1 1 (1)
42	0	0	2	2 2 0 0 (0)
43	0	0	3	0 0 3 3 (0)
44	0	0	3	1 1 2 2 (0)
45	0	0	3	1 1 2 2 (1)
46	0	0	3	2 2 1 1 (0)
47	0	0	3	2 2 1 1 (1)
48	0	0	3	3 3 0 0 (0)
49	0	0	4	1 1 3 3 (0)
50	0	0	4	2 2 2 2 (0)
51	0	0	4	2 2 2 2 (1)
52	0	0	4	3 3 1 1 (0)
53	0	0	5	2 2 3 3 (0)
54	0	0	5	3 3 2 2 (0)
55	0	0	6	3 3 3 3 (0)

	B	I	m	quark state $\bar{u}u\bar{d}d$
56	0	1	1	0 1 1 0 (0)
57	0	1	2	0 1 2 1 (0)
58	0	1	2	1 2 1 0 (0)
59	0	1	3	0 1 3 2 (0)
60	0	1	3	1 2 2 1 (0)
61	0	1	3	1 2 2 1 (1)
62	0	1	3	2 3 1 0 (0)
63	0	1	4	1 2 3 2 (0)
64	0	1	4	2 3 2 1 (0)
65	0	1	5	2 3 3 2 (0)
66	0	2	2	0 2 2 0 (0)
67	0	2	3	0 2 3 1 (0)
68	0	2	3	1 3 2 0 (0)
69	0	2	4	1 3 3 1 (0)
70	0	3	3	0 3 3 0 (0)

	B	I	m	quark state $\bar{u}u\bar{d}d$
71	1	-3/2	0	0 0 0 3 (0)
72	1	-3/2	1	1 1 0 3 (0)
73	1	-3/2	2	2 2 0 3 (0)
74	1	-3/2	3	3 3 0 3 (0)
75	1	-1/2	0	0 1 0 2 (0)
76	1	-1/2	1	0 1 1 3 (0)
77	1	-1/2	1	1 2 0 2 (0)
78	1	-1/2	2	1 2 1 3 (0)
79	1	-1/2	2	2 3 0 2 (0)
80	1	-1/2	3	2 3 1 3 (0)
81	1	1/2	0	0 2 0 1 (0)
82	1	1/2	1	0 2 1 2 (0)
83	1	1/2	1	1 3 0 1 (0)
84	1	1/2	2	0 2 2 3 (0)
85	1	1/2	2	1 3 1 2 (0)
86	1	1/2	3	1 3 2 3 (0)
87	1	3/2	0	0 3 0 0 (0)
88	1	3/2	1	0 3 1 1 (0)
89	1	3/2	2	0 3 2 2 (0)
90	1	3/2	3	0 3 3 3 (0)
91	2	0	0	0 3 0 3 (0)

- requires additional index in QMC simulations!

Static Limit for $N_{\mathrm{f}} = 2$:

Static limit: $Z = Z_1^V$ with Z_1 is 1-dim QCD partition function

- in the chiral limit, all states $\mathfrak{h} \in \mathbb{H}_{\mathfrak{h}}$ contribute with a weight 1:

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

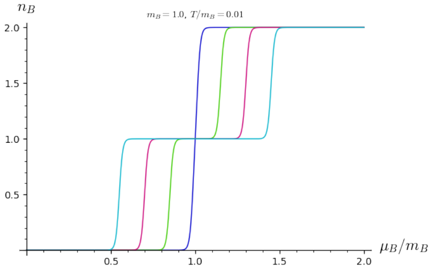
- af finite quark mass: via Conrey-Farmer-Zirnbauer formula

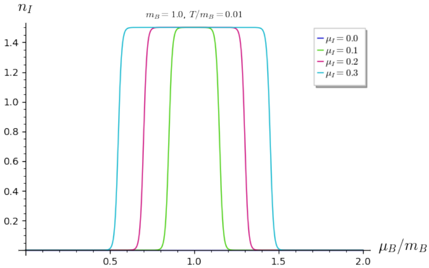
[Ravgali, Verbaarschot, PRD 76 (2007)]

- for degenerate quark mass $m \equiv m_u = m_d$, with $\mu_c = \mu_c(m)$:

$$\mathcal{Z}\left(\frac{\mu_B}{T}, \frac{\mu_I}{T}, \frac{\mu_c}{T}\right) = 2\cosh\frac{3\mu_I}{T} + 4\left(\cosh\frac{\mu_c}{T}\right)^2\left(3 + 2\cosh\frac{4\mu_c}{T} + 2\cosh\frac{2\mu_I}{T}\right) + 4\cosh\frac{\mu_I}{T}\left(2 + 2\cosh\frac{2\mu_c}{T} + \cosh\frac{4\mu_c}{T}\right) + 8\cosh\frac{\mu_B}{T}\left(2\cosh\frac{\frac{3}{2}\mu_I}{T}\cosh\frac{\mu_c}{T} + \cosh\frac{\frac{1}{2}\mu_I}{T}\left(2\cosh\frac{2\mu_c}{T} + 1\right)\right) + 2\cosh\frac{2\mu_B}{T}$$

- for non-zero isospin chemical potential: baryon density has two transitions at low T
- as $n_B = 2$, the isospin density vanishes (Pauli saturation)
- similar finding as in Mean Field for strong coupling limit





Setup of the QMC Simulations

QMC is realized as **Diagrammatic Monte Carlo** (continuous time version of the Worm algorithm):

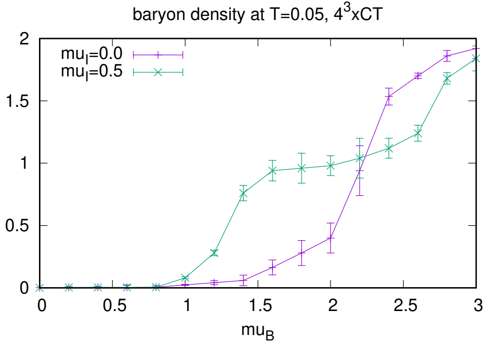
- as for $N_\mathrm{f} = 1$, a continuous Euclidean time Worm algorithm operates on the meson occupation numbers
  1. move update: choose Worm head/tail for specific meson charge $Q = \bar{q}_1 q_2$, only accept if Q can be raised/lowered
  2. shift update: move in temporal direction until pion is emitted/absorbed according to $J^\dagger_{Q,x} J_{Q,y}$, proportional to exponential decay $p(\Delta t) = e^{-\lambda \Delta t}$ with decay constant $\lambda = d_Q(\vec{x})/4T$
  3. repeat [2] until Worm closes

New physics expected:

- single baryons can now coexist with pions, resulting in **pion exchange** between nucleons
- **pion condensation** competes with nuclear phase

Preliminary results

- scan in baryon chemical potential at fixed isospin chemical potential:



- status: so far implemented in Python (data structures quite involved)
- modifying existing continuous time Worm in C++ to gain substantial speed up and scan the full phase diagram

Conclusions

Results:

- Hamiltonian formulation also completely **sign problem-free** for $N_\mathrm{f}=2$ (not the case for discrete N_t!)
- Matrix elements for the **creation and annihilation operators** $\hat{J}^{\pm}$ have now been determined for $N_\mathrm{f}=2,3$
- First exploratory QMC simulations at $\mu_B>0$, $\mu_I>0$,

Goals:

- Determine the phase diagram in the T,μ_B,μ_I-space
- Measure nuclear potential to study pion exchange
- Include gauge corrections also for $N_\mathrm{f}=2$

Interpretation:

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

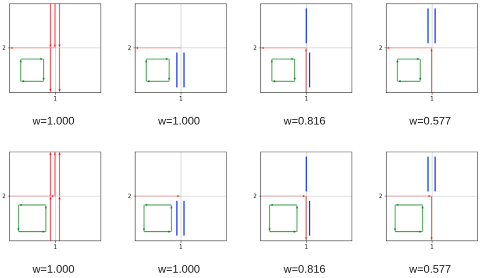
$$\hat{J}_1 = \frac{\sqrt{N_\mathrm{c}}}{2}\left(\hat{J}^+ + \hat{J}^-\right), \quad \hat{J}_2 = \frac{\sqrt{N_\mathrm{c}}}{2i}\left(\hat{J}^+ - \hat{J}^-\right),$$
$$\hat{J}_3 = i[J_1, J_2] = \frac{N_\mathrm{c}}{2}[\hat{J}^+, \hat{J}^-], \quad \hat{J}^2 = \frac{N_\mathrm{c}(N_\mathrm{c}+2)}{4}$$

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

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

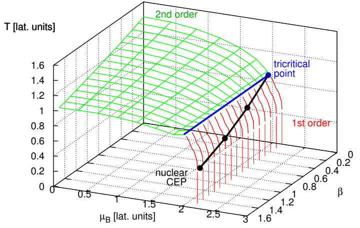
$$\hat{J}^2 \left| \frac{N_\mathrm{c}}{2} \mathfrak{s} \right\rangle = \frac{N_\mathrm{c}\left(N_\mathrm{c}+2\right)}{4} \left| \frac{N_\mathrm{c}}{2}, \mathfrak{s} \right\rangle, \qquad [\hat{J}^2, \hat{J}_3] = 0.$$

- 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 meson exchange, but also allows to **couple baryons!** ($\hat{J}^{\pm}$ still block-diagonal)

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), $N_\mathrm{f} = 1$
- front plane: continuum phase diagram ($\beta = \infty$, $a = 0$), $N_\mathrm{f} = 4$ (no rooting)