The phase diagram at finite baryon and isospin densities at strong coupling

Wolfgang Unger, Bielefeld University

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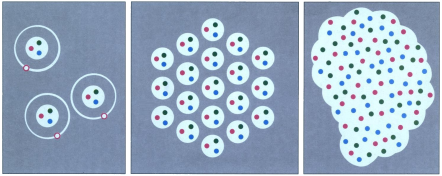


UNIVERSITÄT BIELEFELD

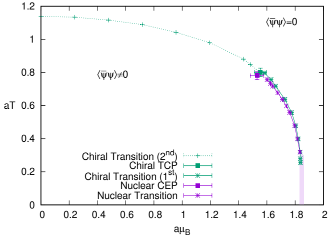
Faculty of Physics

CRC-TR 211 Strong-interaction matter under extreme conditions

2023 LATTICE

Outline

- **Quantum Hamiltonian for 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, CP established [Klegrewe, U. PRD 102 (2020)]



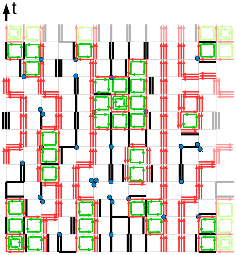
Aim: $N_\mathrm{f} = 2$: Determine the phase diagram for **both finite baryon and isospin chemical potential**

Content of the talk:

1. The Hamiltonian approach to Lattice QCD via Dual Variables
2. Setup of the $N_\mathrm{f} = 2$ Quantum Monte Carlo Simulation
3. Numerical results for finite μ_B, μ_I
4. Outlook on Quantum Computing

Lattice QCD in a Dual Formulation

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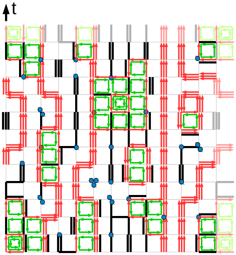
  - at $\beta > 0$: color singlets may include gluon contributions [Gagliardi, U, PRD 101 (2020)]
- Sign problem in regime $\beta = \frac{6}{g^2} \lesssim 1$ **mild enough** to study full phase diagram:
  - baryons are heavy: $\Delta f \simeq 10^{-5}$
  - in continuous time limit $N_t \to \infty$: **baryons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

  $\Rightarrow$ finite density sign problem absent!



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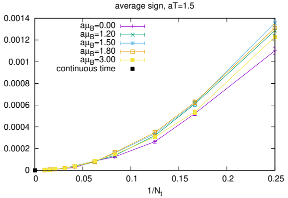
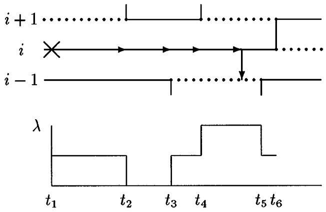


average sign vanishes for $N_t \to \infty$ $(a_t \to 0)$

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

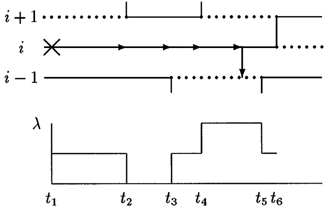
Continuous time (CT) methods

- make time direction continuous: $t \in [0, \beta]$
- sample $Z(\beta) = \mathrm{Tr}[e^{\beta \hat{H}}]$ in terms of **decay probabilities**
  [Beard & Wiese, PRL 77 (1996) 5132]



Euclidean Continuous Time Limit

Continuous time (CT) methods



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Many applications:

- in condensed matter (SSE, Worm) [Gull *et al* (2010)]
- fermion bags approach [Huffman & Chandrasekharan (2020)]

For Strong Coupling LQCD:

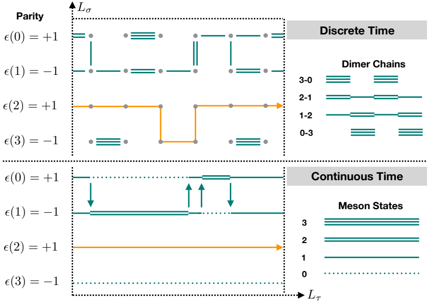
- Introduce **bare anisotropy** γ such that $\xi = \frac{a_s}{a_t} \neq 1$:
- Non-perturbative result: $\xi(\gamma) \approx \kappa\gamma^2 + \frac{\gamma^2}{1+\lambda\gamma^4}, \quad \kappa = 0.781(1)$
  [de Forcrand, Vairinhos, U., PRD 97 (2018)]
- Define the **continuous Euclidean time limit** (CT-limit):

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

From Dimers to Meson Occupation Numbers ($N_f = 1$)

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 $\langle x, y \rangle$

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

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

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

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

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

- **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 $[\hat{\mathcal{H}}, \hat{\mathcal{N}}] = 0$

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

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

- due to continuous time limit, also for $N_\mathrm{f} > 1$, **only single mesons are interchanged** between nearest
- 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!**

Hadronic States for $N_\mathrm{f} = 2$

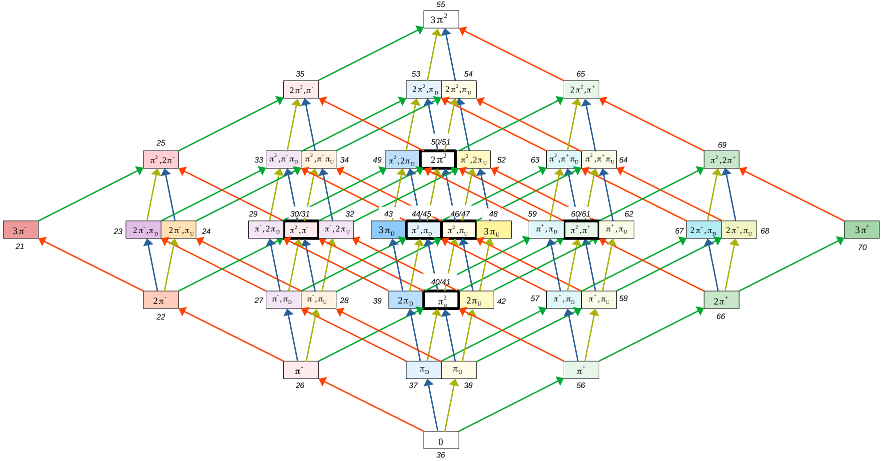
Local Hilbert space $\mathbb{H}_\mathfrak{h}$:

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

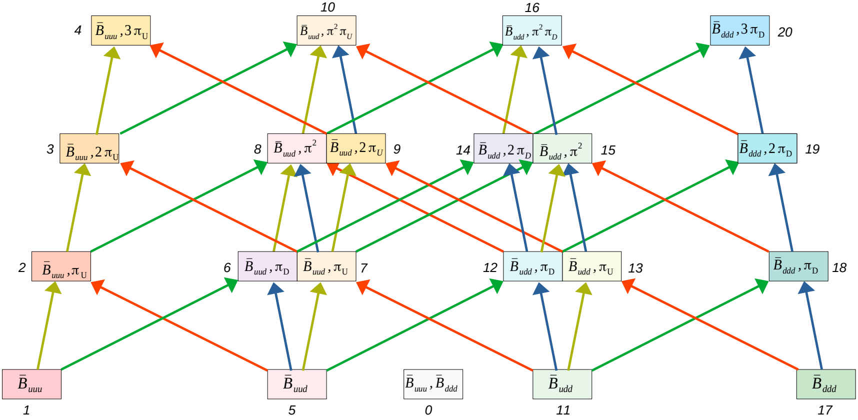
B	I	$\mathfrak{m}=0$	$\mathfrak{m}=1$	$\mathfrak{m}=2$	$\mathfrak{m}=3$	$\mathfrak{m}=4$	$\mathfrak{m}=5$	$\mathfrak{m}=6$	Σ
-2	0	1							1
-2	Σ	1	0	0	0	0	0	0	1
-1	$-\frac{3}{2}$	1	1	1	1				4
-1	$-\frac{1}{2}$	1	2	2	1				6
-1	$+\frac{1}{2}$	1	2	2	1				6
-1	$+\frac{3}{2}$	1	1	1	1				4
-1	Σ	4	6	6	4	0	0	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

Transitions between states: $B = 0$

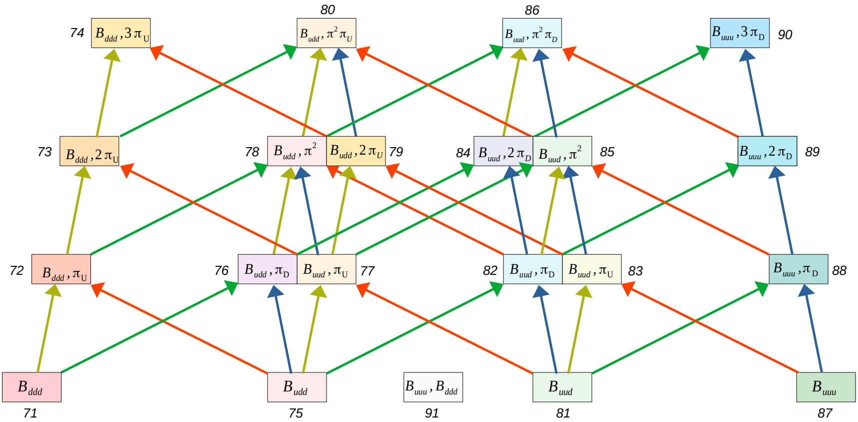
- states only distinguishable on quark level, eg. $\pi_+\pi_- = \pi_U\pi_D \equiv \pi^2$
- quark content not sufficient, some states have twofold degeneracy:



Transitions between states: $B = -1, -2$

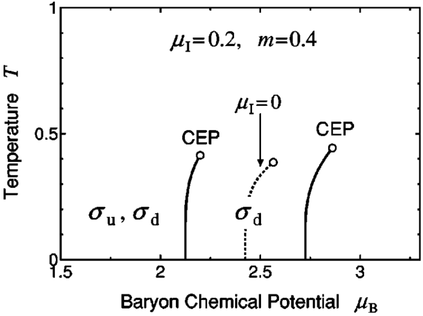


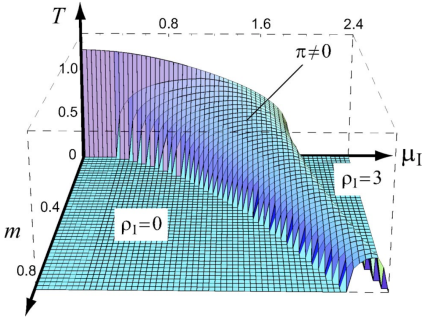
Transitions between states: $B = 1, 2$



Expectations from Mean Field Theory at Strong Coupling ($N_\mathrm{f} = 2$)

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



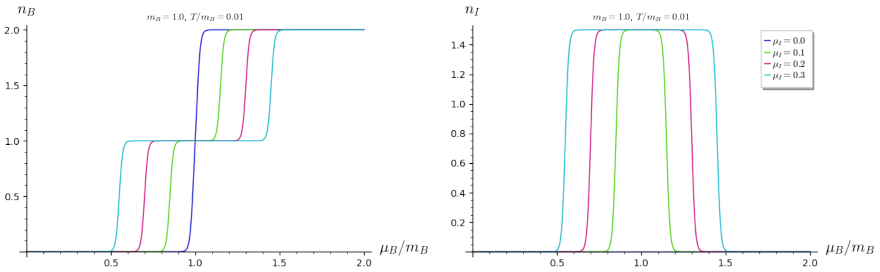


[Nishida, PRD **69 (2004)**]

- Continuum extrapolated $N_\mathrm{f} = 2 + 1$ QCD phase diagram at non-zero μ_I, but $\mu_B = 0$ shows pion condensation [Brandt et al., Confinement 2018 (260)]

Analytic results in the Static Limit: Finite Quark Mass

- 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

As for $N_\mathrm{f} = 1$, a continuous Euclidean time **Worm algorithm** operates on the **meson occupation numbers**:

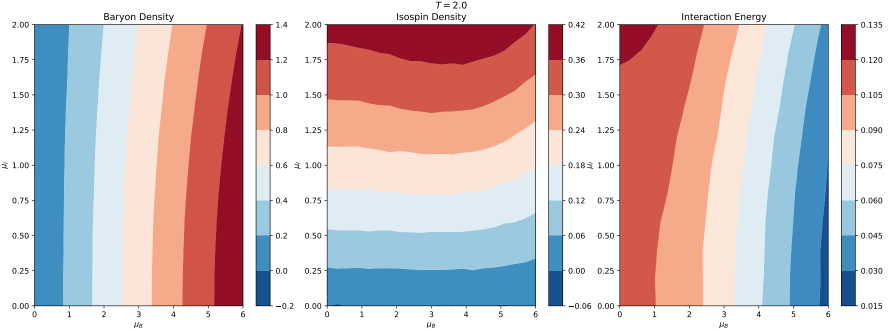
1. move update: choose Worm head/tail for specific meson charge $Q = \bar{q}_1 q_2$, only accept if Q can be raised/lowered
2. shift update: move in temporal direction until pion is emitted/absorbed according to $J^\dagger_{Q,x} J_{Q,y}$, proportional to exponential decay $p(\Delta t) = e^{-\lambda \Delta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

<u>New physics expected:</u>

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

Thermodynamic Observables in chiral limit

- baryon density: **nuclear transition** at $\langle n_B \rangle \simeq 1$ for $T < 1.0$, **Pauli saturation** at $\langle n_B \rangle = 2$
- isospin density: $\langle n_I \rangle$ only non-zero in the nuclear transition region, vanishing in the chirally broken and Pauli saturated phase
- interaction energy: pion exchange, measure for **chiral symmetry breaking**
- μ_B-μ_I-plane for various temperatures T:



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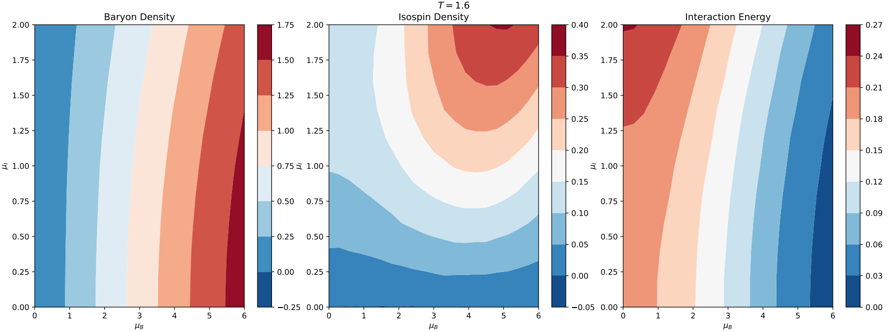

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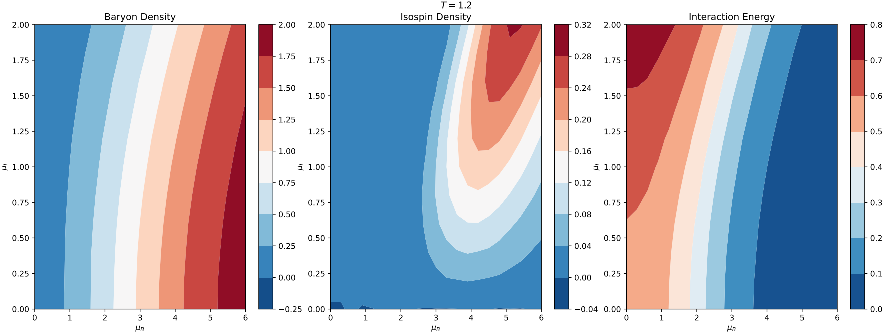

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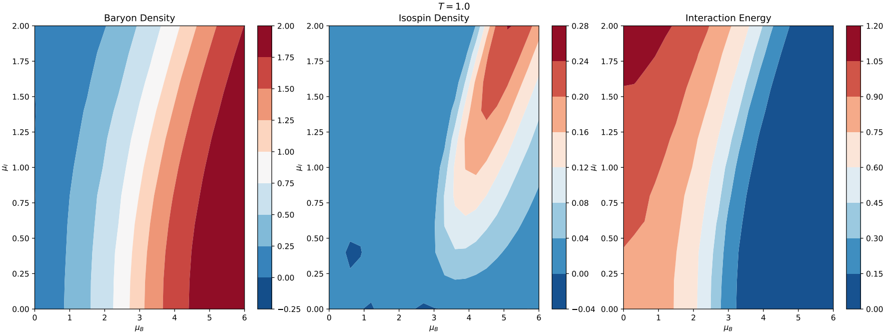

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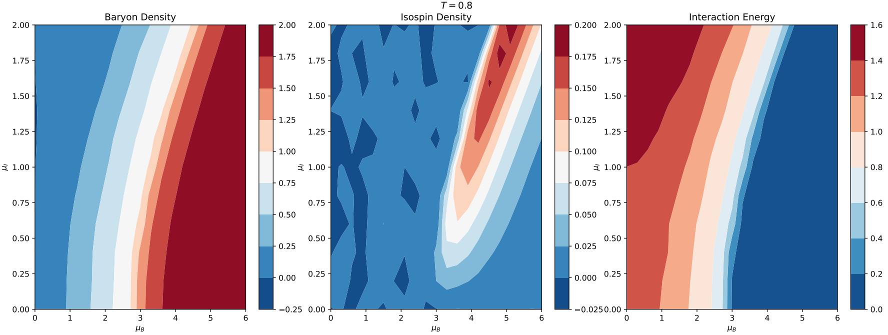

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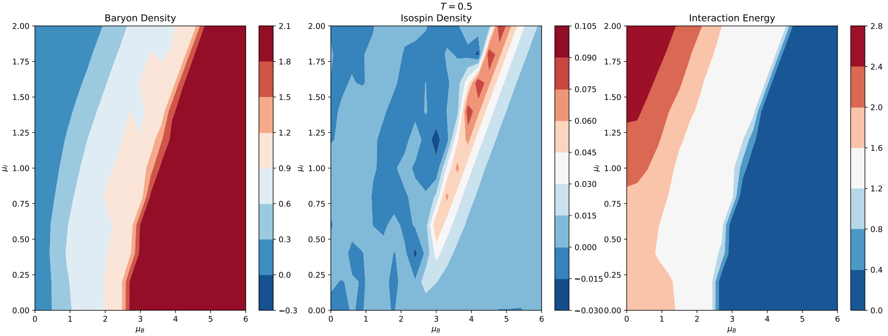

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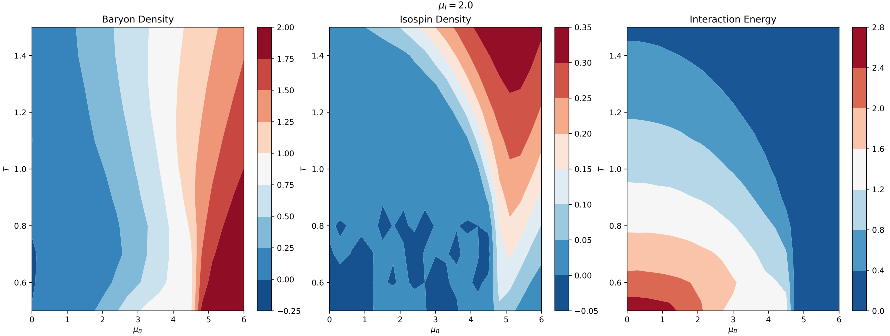

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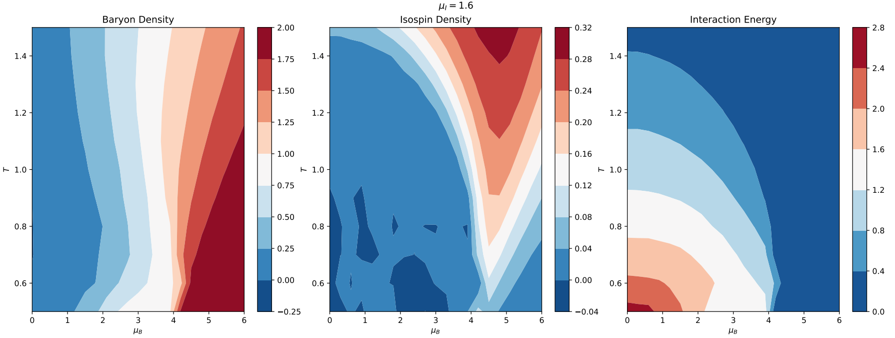

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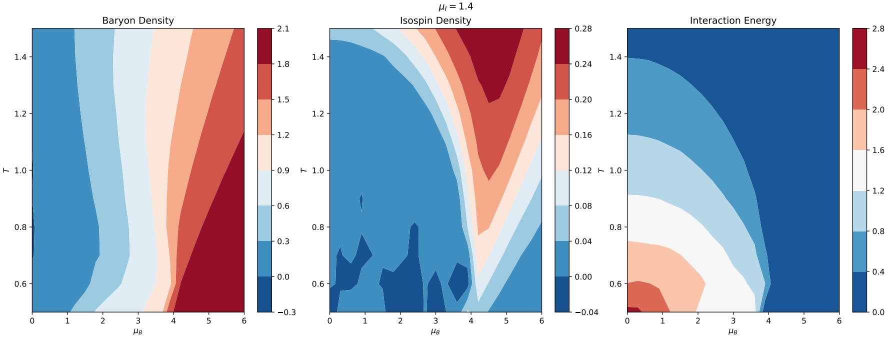

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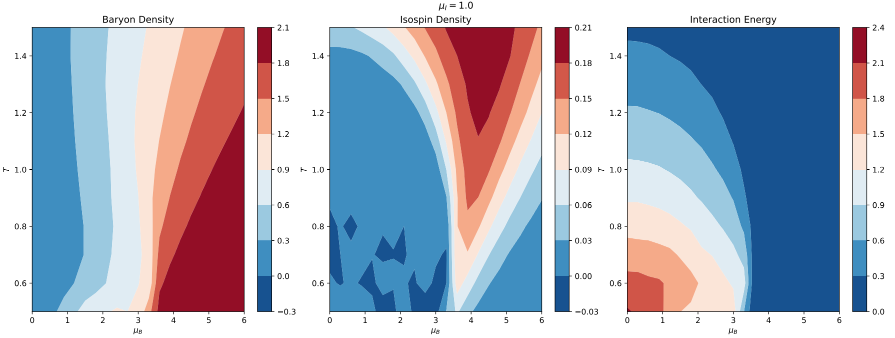

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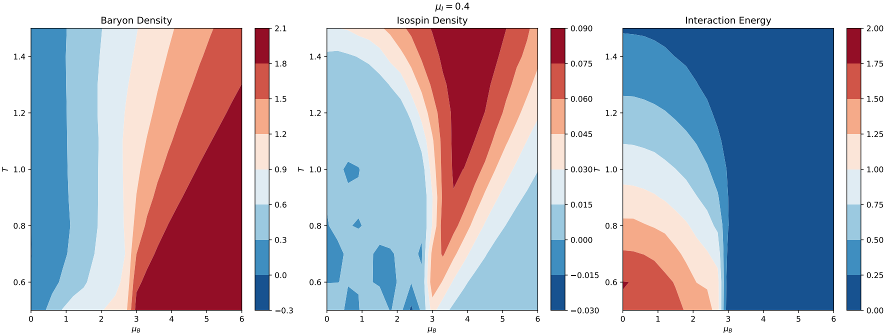

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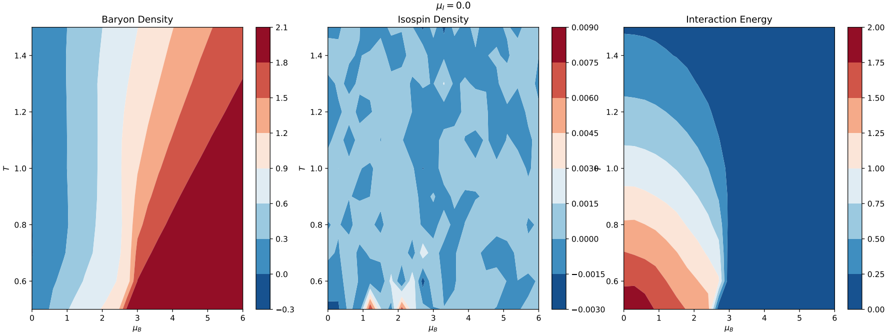
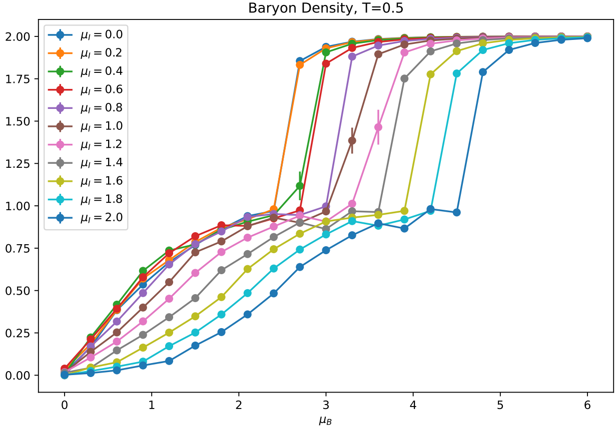


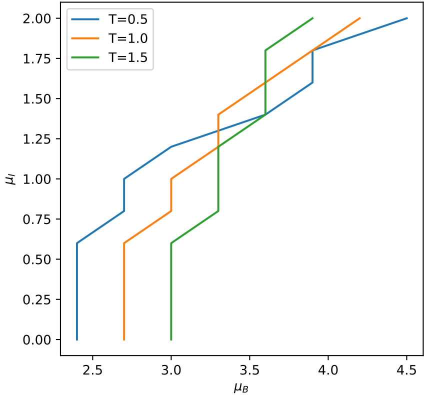
Two transitions?

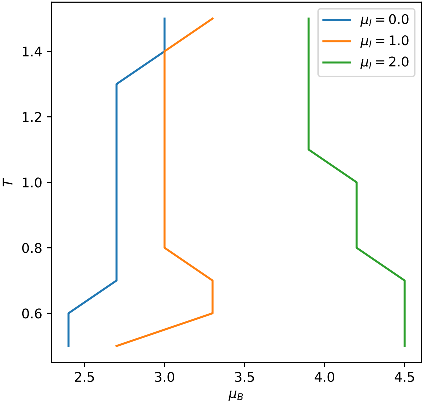
- lowest temperature so far: $T = 0.5$, which has a first order nuclear transition
- no plateau found at $\langle n_B \rangle = 1$, but two regimes are visibile
- lower temperatures might be required (but computationally expensive)



Phase Diagram

- nuclear transition μ_B^c depends strongly on μ_I, weakly on T





- location of CEP not yet established: all data based on 8^3 volume
- finite size scaling using isospin and baryon susceptibilities on the way

Developing an algorithm for gate-based quantum computing

Map the quantum Hamiltonian on **quantum circuits:**

[with M. Fromm, C. Winterowd, O. Philipsen, in preparation]

- degrees of freedom already discrete, **can be easily qubitzed**
- Gauss law is not an issue, can be readily applied to 3 spatial dimensions
- for $N_{\mathrm{f}} = 1$, $\mathrm{U}(3)$: 2 by 2 qubit coupling, four families of set of commuting Pauli strings, for which quantum circuits have been derived
- for $\mathrm{SU}(3)$, an additional qubit is required to capture the static baryons
- for $N_{\mathrm{f}} = 2$, we requires a 6 by 6 qubit coupling for $\mathrm{U}(3)$, not yet fully analyzed for $\mathrm{SU}(3)$

For strong coupling lattice QCD on a quantum annealer:

$\rightarrow$ **talk by Jangho Kim, Wed. 9:00, Quantum Computing Session**

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 $N_\mathrm{f} = 2, 3$
- via continuous time worm algorithm:
  - determined the phase diagram in the T, μ_B, μ_I-space
  - finding similar to expectation from meanfield
- first steps towards Quantum Computing

Further Goals:

- measure nuclear potential to study pion exchange
- include gauge corrections also for $N_\mathrm{f} = 2$

For gauge corrections for $N_\mathrm{f} = 1$:
$\rightarrow$ **talk by Pratitee Pattanaik, Wed. 9:20, Finite Temperature Session**