Continuous Time Monte Carlo for QCD in the Strong Coupling Limit

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and Philippe de Forcrand, ETH Zürich/CERN

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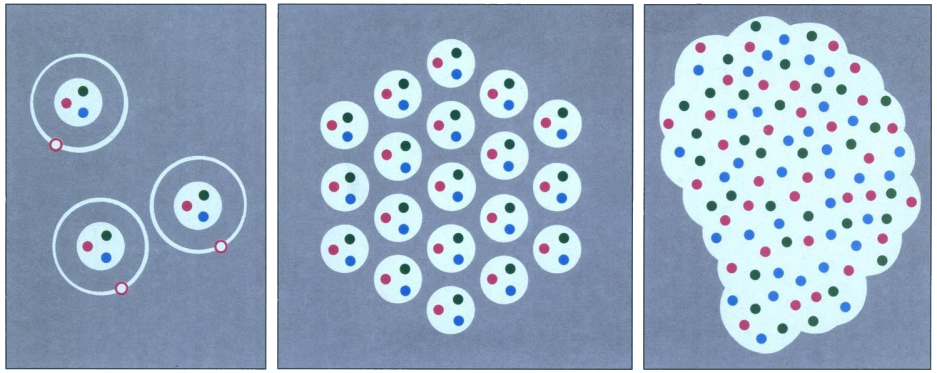

Eidgenössische Technische Hochschule Zürich
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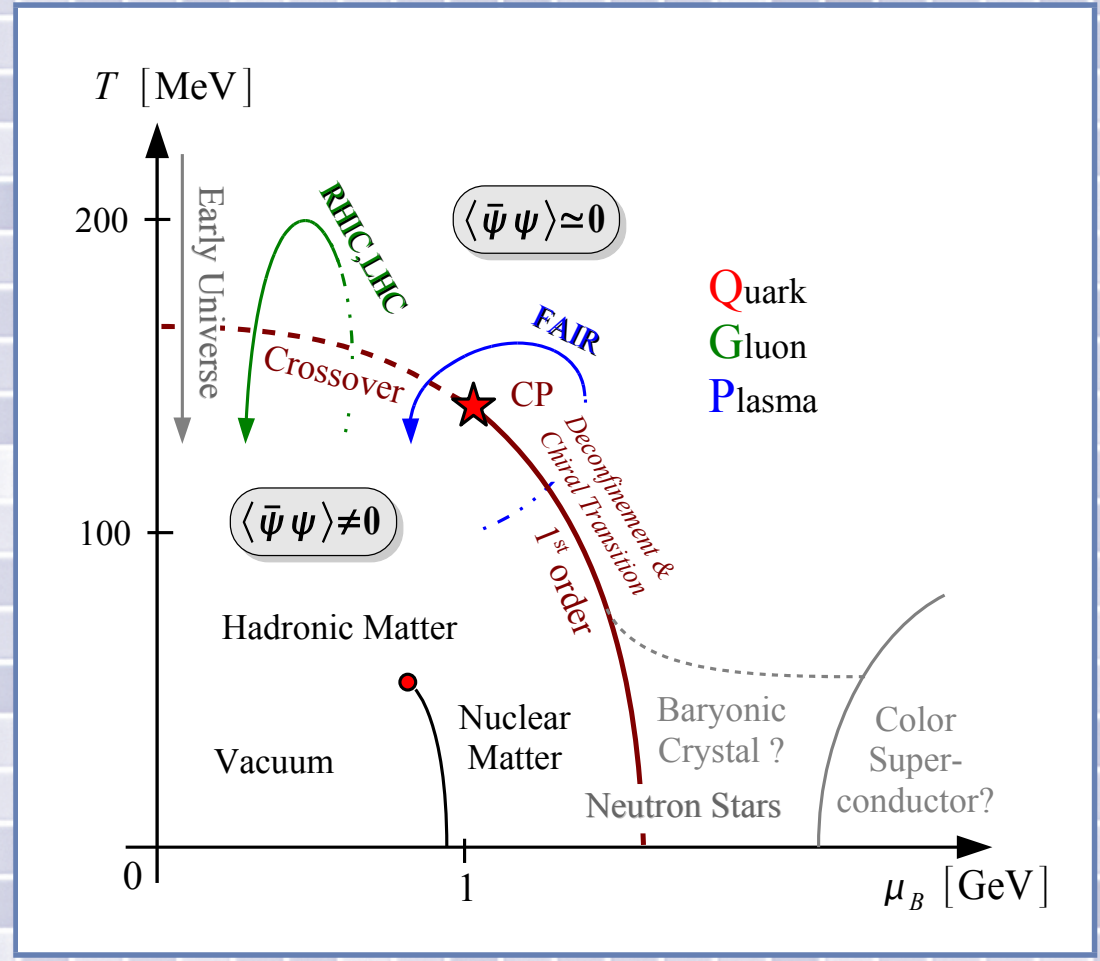
Motivation for Strong Coupling QCD

QCD Phase Diagram

- QCD Phase Diagram: long-standing problem is the location of the CP
- Conjectured Phase Diagram: rich phase structure



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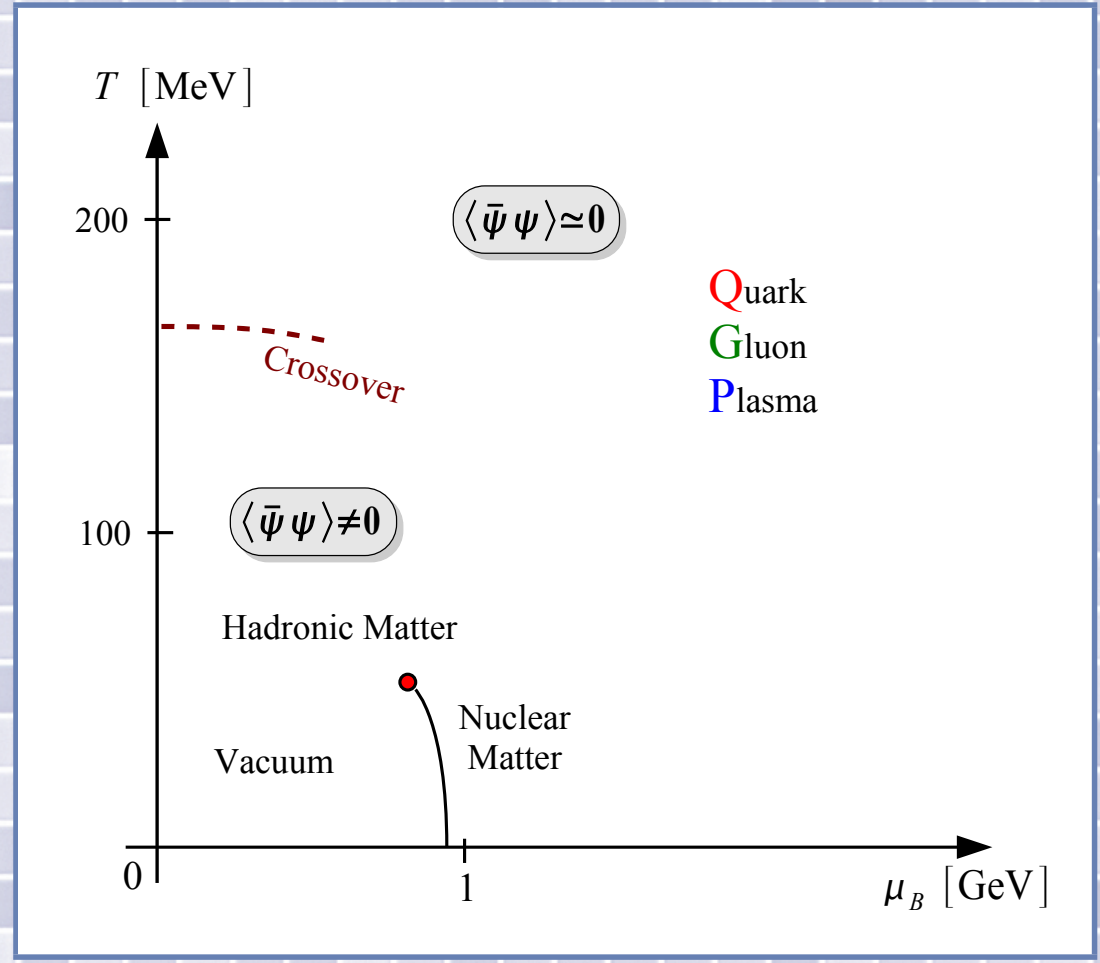
- What we actually know so far: very little



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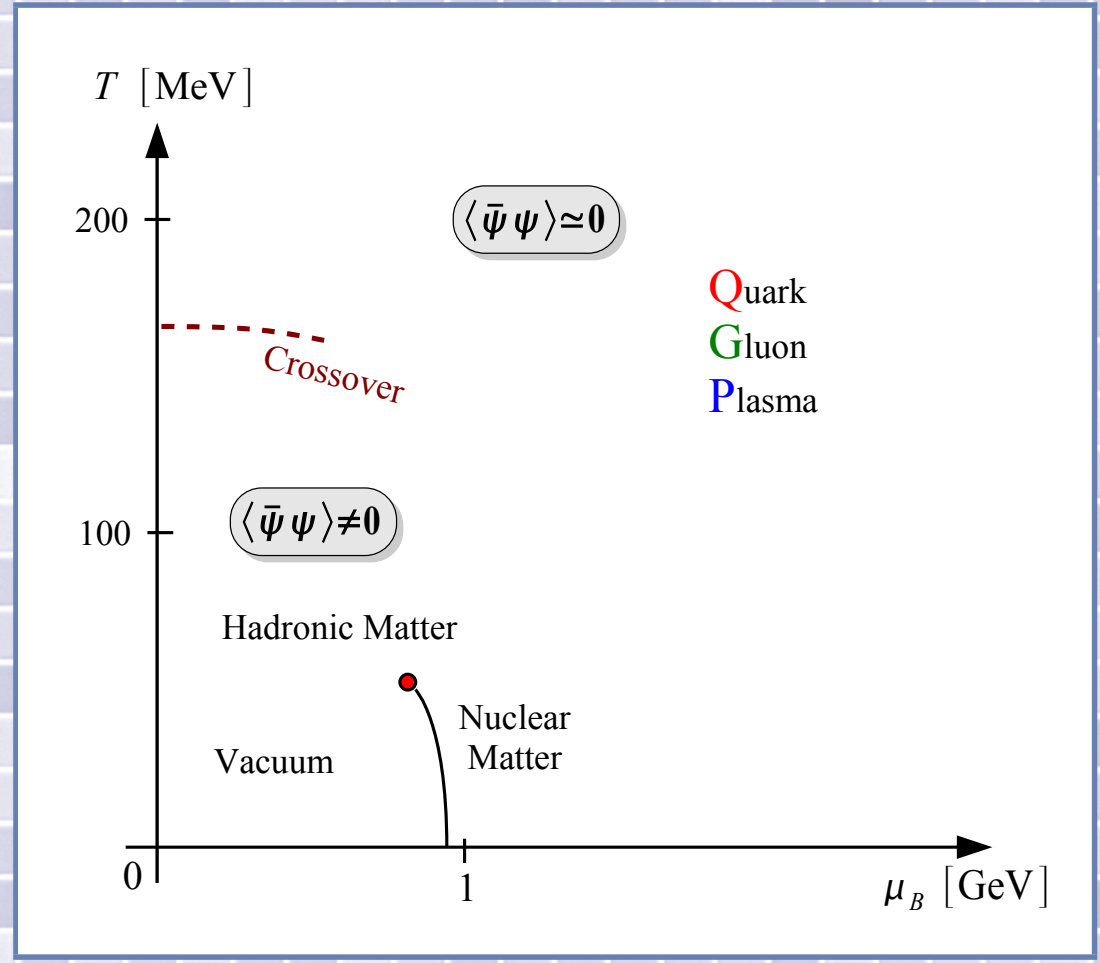

Strong Coupling QCD might help to unravel the phase diagram

Why Study Strong Coupling QCD on the Lattice?

The trouble: the **sign problem** in Lattice QCD

- in Monte Carlo simulations: weight in partition function has to be positive to allow for **importance sampling**
- QCD with finite chemical potential μ: fermion determinant of fermion matrix $M(\mu) = \not{D} + m\mathbb{1} + \mu\gamma_0$ becomes **complex!**
  - quarks anti-commute, integrate them out $\Rightarrow$ $\exp(-S_f) = \det M(\mu)$
  - $\gamma_5(i\not{p} + m + \mu\gamma_0)\gamma_5 = (i\not{p} + m + \mu\gamma_0)^\dagger$ $\Rightarrow$ $\det M(\mu) = \det^* M(-\mu^*)$
- little hope that it can be circumvented, instead: try imaginary μ with analytic continuation, reweighting, Taylor expansion (all **limited to small** $\mu/T \lesssim 1$)

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Strong Coupling QCD circumvents the problem:

- instead of integrating over fermions (HMC): integrate over gauge links U_μ first
- the **sign problem** becomes **mild!**
- allows to study the phase diagram for arbitrarily large chemical potential

What is Strong Coupling QCD?

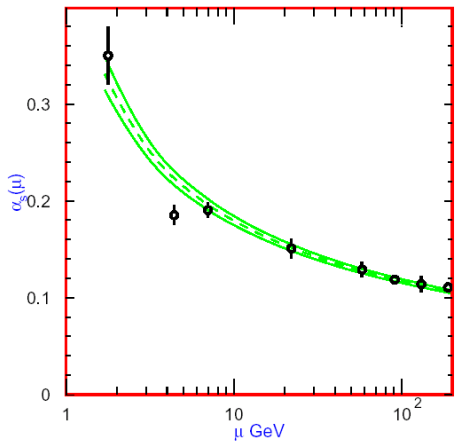
QCD in the strong coupling limit: effective theory for **nuclear matter**

- start from the (1-flavor) QCD Lagrangian in Euclidean time:

$$\mathcal{L}_{\mathrm{QCD}} = \bar{\psi}\left(\gamma_\mu[\partial_\mu + igA^a_\mu t^a] + m_q\right)\psi - \cancel{\frac{\beta}{2N_c}\sum_P \left(\mathrm{tr}\,U_P + \mathrm{tr}\,U_P^\dagger\right) + \mathcal{O}(a^2)}$$

- send the **gauge coupling to infinity:**

$$g \to \infty \quad \Rightarrow \quad \beta = \frac{2N_c}{g^2} \to 0$$



- allows to integrate out the gauge fields completely!
- converse to asymptotic freedom:
  $a(\beta) \sim \exp\left(-\beta/4N_c b_0\right)$
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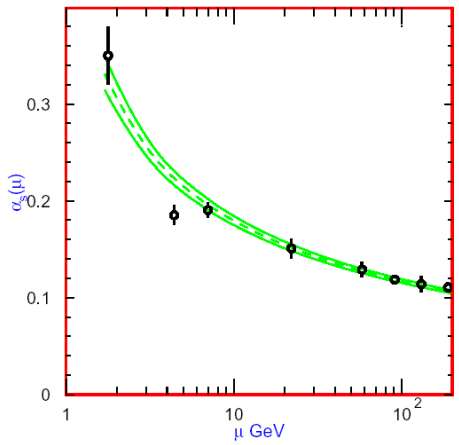

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1-flavor strong coupling QCD might appear crude, but:

- exhibits also **confinement** (only color singlet degrees of freedom)
- and **chiral symmetry breaking** ($U_A(1)$ spontaneously broken below T_c)

Partition function of SC-LQCD with staggered fermions

Key step: **link integration factorizes:** $\int [dU] = \int \prod_{x,\mu} dU_\mu$,

one-link integral can be done analytically.

New degrees of freedom (exact rewriting of QCD path integral, once β is set to zero!)

- Monomers correspond to mesons: $M(x) = \bar{\psi}(x)\psi(x)$
- Dimers correspond to meson hoppings (non-oriented): $k_\mu(x) \in \{0, 1, \ldots, 3\}$
- Baryons $B(x) = \frac{1}{3}\epsilon_{i_1 \ldots i_3}\chi_{i_1}(x)\ldots\chi_{i_3}(x)$ form self-avoiding oriented loops:

$\bar{B}(x)B(y) \in 0, 1$ and $\rho(x,y) = \eta_{\hat{\mu}}(x)\left(\gamma \exp\left(\pm a_t \mu\right)\delta_{\hat{\mu}\hat{0}} + (1 - \delta_{\hat{\mu}\hat{0}})\right)$

Partition function of SC-LQCD with staggered fermions

Integrating out the fermion fields (Grassmann integrals) leads to the **Strong Coupling Partition Function**:

$$\mathcal{Z}(m,\mu_q) = \sum_{\{k,n,l\}} \prod_{b=(x,\hat{\mu})} \frac{(3-k_b)!}{3!k_b!}\gamma^{2k_b\delta_{\hat{0}\hat{\mu}}} \prod_x \frac{3!}{n_x!}(2am_q)^{n_x} \prod_l w(l)$$

- with Grassmann constraint (color neutral states at each lattice site)
  - for mesons:

$$n_x + \sum_{\hat{\mu}=\pm\hat{0},\ldots\pm\hat{d}} k_{\hat{\mu}} = 3 \quad \forall x \in C$$

- weight for baryon loops:

$$w(l) = \left(\prod_{x\in l} 3!\right)^{-1} \sigma(l)\gamma^{3N_{\hat{0}}}\exp\left(3N_\tau r_l a_t \mu\right)$$

Algorithms for SC-LQCD

First: Monte Carlo with **MDP Algorithm**
(Karsch & Mütter, *Nucl. Phys B13 (1989)*)

- trades dimers for monomer pairs, polymers for baryon loops
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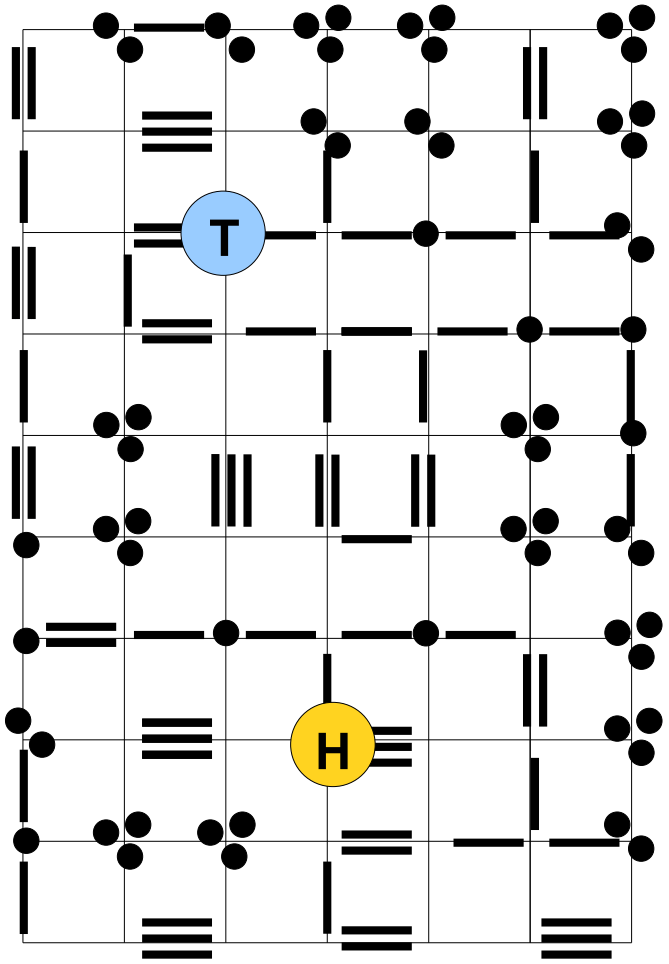
Improvement: **Worm Algorithm!** (Prokof'ev & Svistunov, *Phys. Lett. A238 (1998)*)

- enlarges space of sampled configurations by relaxing Grassman constraint
- adapted for SC-QCD by Adams & Chandrasekharan, *Nucl. Phys. B662 (2003)*

Algorithmic Details

Idea of worm algorithm: Put a worm's **head** and **tail** at a lattice site as **source** and **sink** for **monomers** and move the worm's head through the lattice until it closes again

- **sample** monomer **correlation function** $G(x, y)$
  $\rightarrow$ obtain monomer (chiral) susceptibility
- worm update is a guided random walk
- sample closed path configurations on which to measure observables, global update



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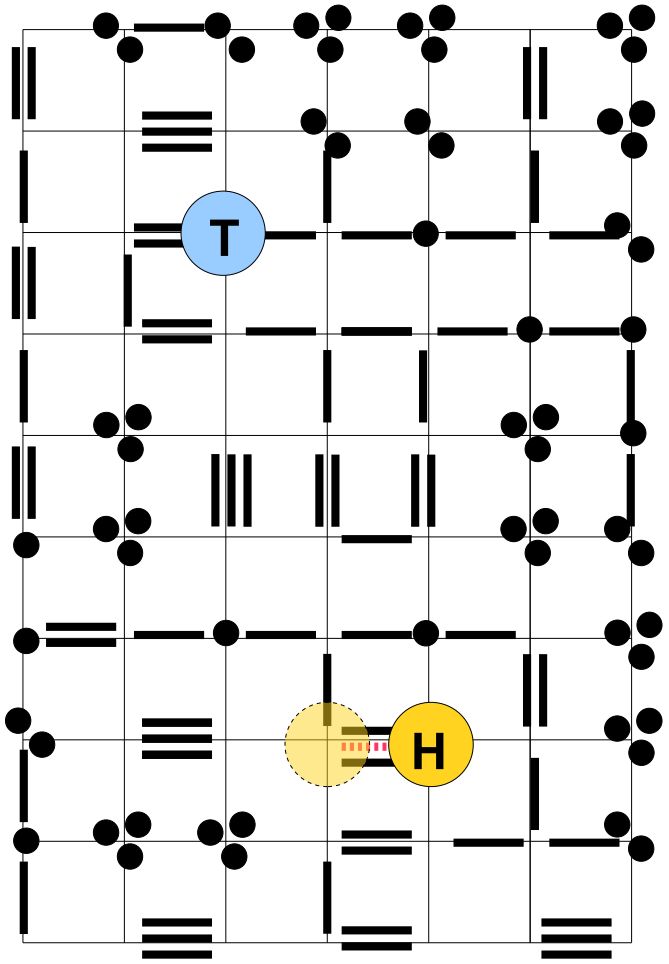

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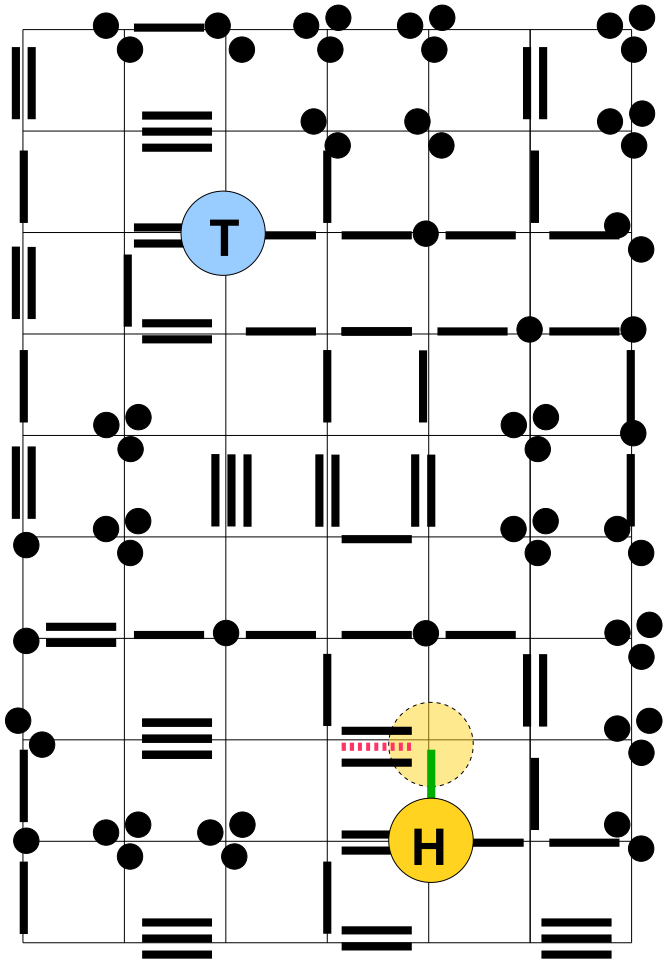

Why continuous time?

Motivation for continuous Euclidean time: **continuum limit**

$N_\tau \to \infty, \gamma^2 \to \infty$ with $aT \simeq \gamma^2/N_\tau$ fixed

- removes cut-off effects in temporal lattice spacing a_t, no extrapolation needed
- resolves ambiguities in the functional dependence $f(\gamma) = \frac{a}{a_t}$
- faster than simulating lattices with $N_\tau > 16$
- continuous temporal correlation functions $G(t, t')$ can be analytically continued

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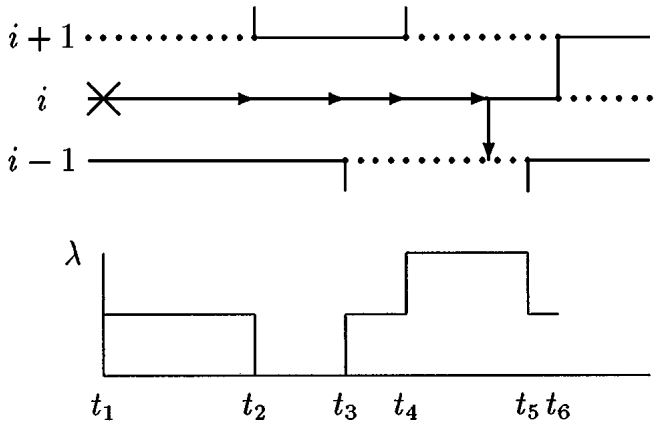
Continuous time first proposed for Quantum Monte Carlo (B. B. Beard & U. J. Wiese, *Phys. Rev. Lett. 77 (1996) 5132*)

1. rewrite the partition function in terms of transition probabilities (decay)
2. make time direction continuous, transitions may occur at any time



Algorithm in Continuous Time Limit

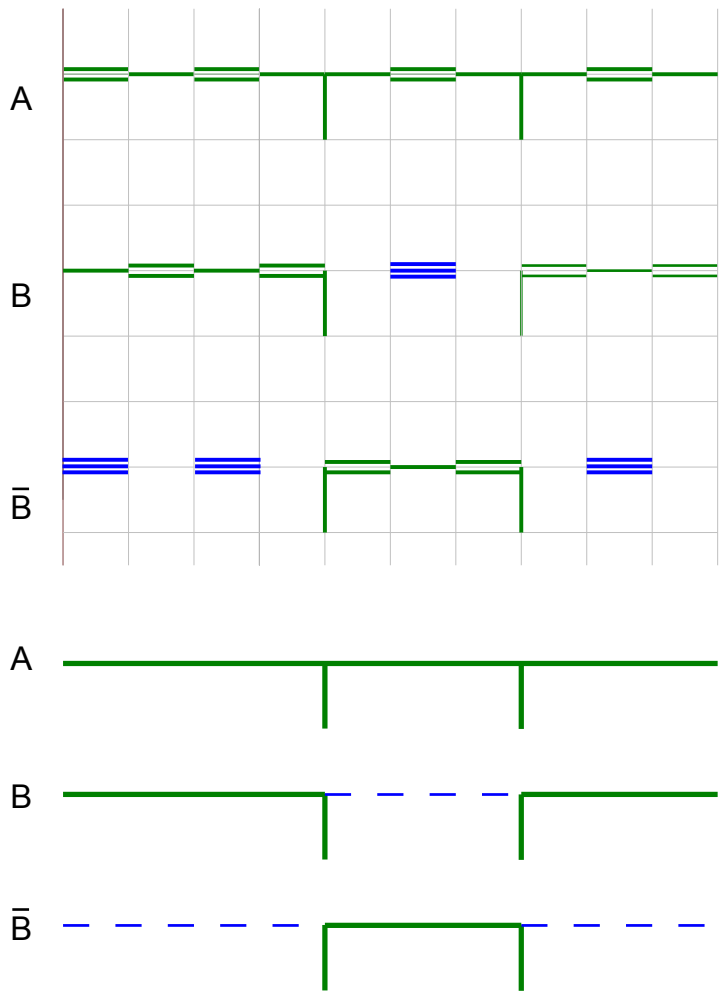
Key observation for SC-QCD: spatial dimers are suppressed in the continuum limit:

- they pick up a factor γ^{-2} from $\mathcal{Z}$
- "decay" probability: **hopping probability**

spatial dimers are rare, temporal dimers form long chains (temporal intervals):

- **dashed lines:** 3-0-3-0-... chains, cannot emit spatial dimers
- **solid lines:** 2-1-2-1-... chains, can emit spatial dimers
- distinguish **L-vertices** (weight $v_L = 1$) and **T-vertices** ($v_T = 2/\sqrt{3}$)

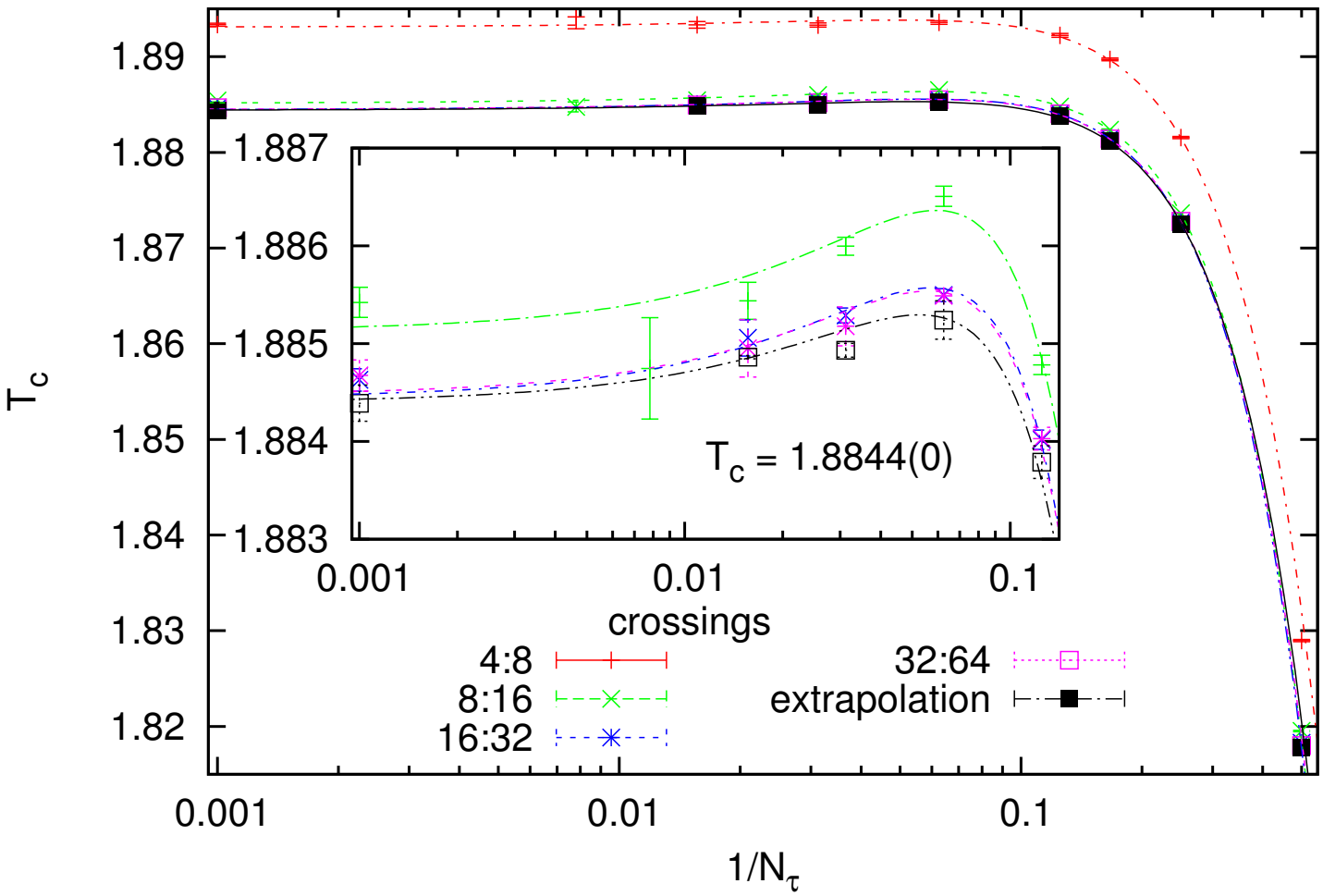
$$\mathcal{Z}(T) = \prod_x v_L^{n_L(x)} v_T^{n_T(x)} \simeq \prod_x 3^{-n_I(x)/2} \prod_i^{n_I(x)} P(\Delta\hat{\beta}_i)$$



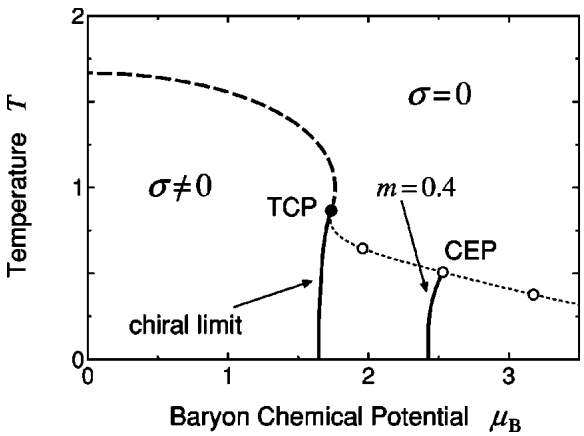
Continuum Extrapolation and Continuous Results

Finite size scaling analysis for O(2) universality class of U(3) transition.

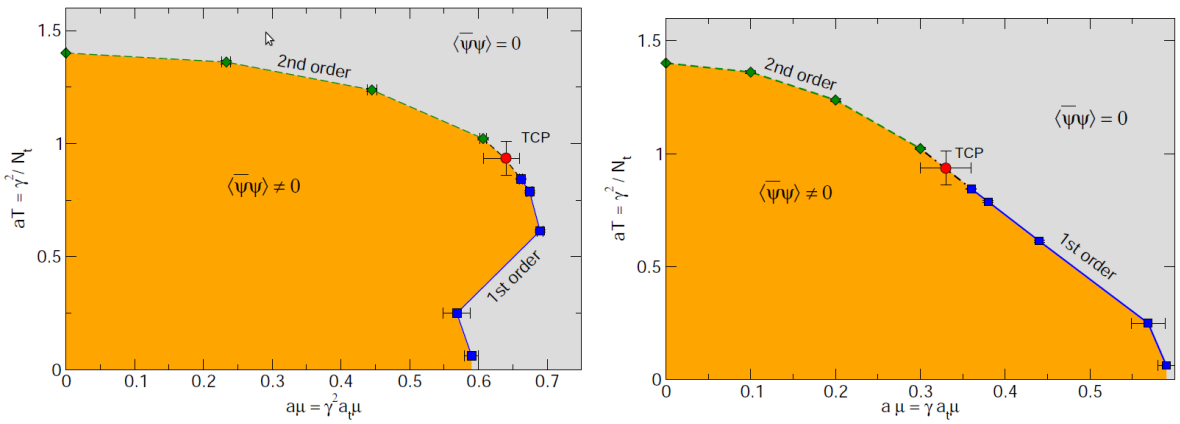
Fit ansatz for pseudo-critical temperatures: $T_{pc}(N_\tau) = T_c + a/N_\tau + b/{N_\tau}^2$



The SU(3) Strong Coupling Phase Diagram (Chiral Limit)



from Y. Nishida, PR D 69 (2004)



from Ph. de Forcrand, M. Fromm, PRL 104 (2010)

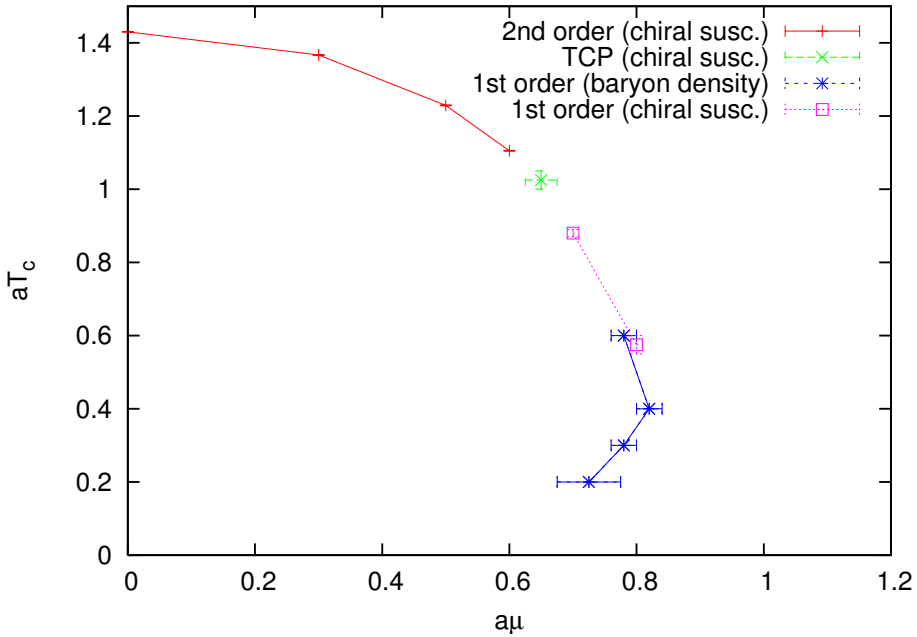
Previous findings in the literature:

- mean field theory of SC-QCD predicts a peculiar behaviour of the first order transition line
- this was indeed found in the simulation, based on the discrete algorithm
- amiguity of the functional dependence of chemical potential μ on anisotropy γ remained

The SU(3) Strong Coupling Phase Diagram (Chiral Limit)

- In the continuum limit: baryon hoppings are suppressed with γ^3

  $\Rightarrow$ **baryons become static**.
- Baryonic worm update simplifies in continuous time, baryons are (dis)favored by a factor $\exp(\pm 3\mu/T)$ over mesons.
- The location of the tricritical point agrees with previous findings.
- At $T = 0$, $\mu^B_{\mathrm{crit}} < M_B$: strong nuclear interactions present (see Ref. [1]).
- Re-entrance seen (the entropy decreases in the high-density phase, due to saturation).



Summary

Main Messages:

- No need to perform continuum extrapolation $N_t \to \infty$. Results in very good agreement with extrapolated discrete data.
- Continuous algorithm faster than discrete algorithm for $N_t = 16$ lattices at T_c.
- The continuum formulation has no sign problem.

Outlook:

- Continuous time correlation functions can be measured and analytically continued.
- Extension to finite quark masses obtained by generating monomers with probability density $\exp(-2m_q\Delta\hat{\beta})$.

Other aspects of SC-QCD:

- Nuclear Physics from Strong Coupling QCD: Michael Fromm, PhD Thesis and *Phys. Rev. Lett. 104 (2010)*
- $\mathcal{O}(\beta)$ corrections (Michael Fromm, Owe Philippsen, Jens Langelage)
- Generalization to $N_\mathrm{f} = 2$