Diagrammatic Monte Carlo for Strong Coupling LQCD

Wolfgang Unger, ETH Zürich with Philippe de Forcrand, ETH Zürich/CERN Yukawa Institute, Kyoto

20.02.2012



ETH

Eidgenössische Technische Hochschule Zürich Swiss Federal Institute of Technology Zurich









• only recently: agreement on crossover temperature *T_c* at zero baryon chemical potential QCD has a severe sign problem for finite chemical potential $\mu = \frac{1}{3}\mu_B$:

• fermions anti-commute:

 $\gamma_5(i\not\!\!p+m+\mu\gamma_0)\gamma_5=(i\not\!\!p+m+\mu\gamma_0)^{\dagger}$

the fermion determinant det M(μ) becomes complex!

 $e^{-S_f} = \det M(\mu) = \overline{\det M(-ar\mu)}$

- little hope that it can be circumvented:
 - Taylor expansion,
 - imaginary μ with analytic continuation,
 - reweighting method

are all limited to small $\mu/T \lesssim 1$

Wolfgang Unger, ETH Zürich

What is Strong Coupling Lattice QCD?

Look at QCD in a regime where the sign problem can be made mild: This is obtained by changing the nature of integration variables:

- no sampling of gauge fields $\{U\}!$
- no fermion determinant (no HMC)!

Staggered QCD in the strong coupling limit:

• start from the "1-flavor" staggered QCD Lagrangian in Euclidean time: $\mathcal{L}_{\rm QCD} = \sum_{\nu} \frac{1}{2} \eta_{\nu}(x) \left(e^{\mu \delta_{\nu 0}} \bar{\chi}(x) U_{\nu}(x) \chi(x+\hat{\nu}) - e^{-\mu \delta_{\nu 0}} \bar{\chi}(x+\hat{\nu}) U_{\nu}^{\dagger}(x) \chi(x) \right) + a m_q \bar{\chi} \chi - \frac{\beta}{2N_c} \sum_{P} \left(\operatorname{tr} U_P + \operatorname{tr} U_P^{\dagger} \right) + \mathcal{O}(a^2)$



What is Strong Coupling Lattice QCD?

Look at QCD in a regime where the **sign problem** can be made mild: This is obtained by changing the nature of integration variables:

- no sampling of gauge fields $\{U\}!$
- no fermion determinant (no HMC)!

Staggered QCD in the strong coupling limit:

• start from the "1-flavor" staggered QCD Lagrangian in Euclidean time: $\mathcal{L}_{\text{QCD}} = \sum_{\nu} \frac{1}{2} \eta_{\nu}(x) \left(e^{\mu \delta_{\nu 0}} \bar{\chi}(x) U_{\nu}(x) \chi(x+\hat{\nu}) - e^{-\mu \delta_{\nu 0}} \bar{\chi}(x+\hat{\nu}) U_{\nu}^{\dagger}(x) \chi(x) \right) + a m_q \bar{\chi} \chi$

$$-\frac{\beta}{2N_{\rm c}}\sum_{P}\left({\rm tr}U_{P}+{\rm tr}U_{P}^{\dagger}\right)+\mathcal{O}(a^{2})$$

• take limit of infinite gauge coupling:

$$g
ightarrow\infty,\;eta=rac{2N_{
m c}}{g^2}
ightarrow 0$$

• allows to integrate out the gauge fields completely, as link integration factorizes

What is Strong Coupling Lattice QCD?

Look at QCD in a regime where the sign problem can be made mild: This is obtained by changing the nature of integration variables:

- no sampling of gauge fields $\{U\}!$
- no fermion determinant (no HMC)!

Staggered QCD in the strong coupling limit:

- start from the "1-flavor" staggered QCD Lagrangian in Euclidean time: $\mathcal{L}_{\text{QCD}} = \sum_{\nu} \frac{1}{2} \eta_{\nu}(x) \left(e^{\mu \delta_{\nu 0}} \bar{\chi}(x) U_{\nu}(x) \chi(x+\hat{\nu}) e^{-\mu \delta_{\nu 0}} \bar{\chi}(x+\hat{\nu}) U_{\nu}^{\dagger}(x) \chi(x) \right) + a m_q \bar{\chi} \chi$
 - $-\frac{\beta}{2N_{\rm c}}\sum_{P}\left({\rm tr}U_{P}+{\rm tr}U_{P}^{\dagger}\right)+\mathcal{O}(a^{2})$
- take limit of infinite gauge coupling:

$$g
ightarrow\infty,\;eta=rac{2N_{
m c}}{g^2}
ightarrow 0$$

• allows to integrate out the gauge fields completely, as link integration factorizes

Drawback: strong coupling limit is converse to asymptotic freedom:

- degrees of freedom in SC-QCD live on a crystal
- fermions have no spin (taste splitting maximal)

Why Strong Coupling Lattice QCD?

1-flavor strong coupling QCD might appear crude, but

- exhibits confinement, i.e. only color singlet degrees of freedom survive:
 - mesons (rep. by monomers and dimers)
 - baryons (rep. by oriented self-avoiding loops)
- and chiral symmetry breaking/restoration:

 $\mathsf{U}_{\mathsf{A}}(1): \qquad \chi(x) \mapsto e^{i\eta_5(x)\theta_{\mathsf{A}}}\chi(x), \ \bar{\chi}(x) \mapsto \bar{\chi}(x)e^{i\eta_5(x)\theta_{\mathsf{A}}}, \qquad \eta_5(x)e^{i\eta_5(x)\theta_{\mathsf{A}}},$

$$\Sigma_{5}(x) = (-1)^{\sum_{\nu=0}^{d} x_{\nu}}$$

is spontaneously broken below T_c ,

hence its phase diagram might be similar to the QCD phase diagram

SC-LQCD as effective theory for nuclear matter:

- derive nuclear interactions between hadrons from (Lattice) QCD
- transition at high density is the nuclear transition

Why Strong Coupling Lattice QCD?

1-flavor strong coupling QCD might appear crude, but

- exhibits confinement, i.e. only color singlet degrees of freedom survive:
 - mesons (rep. by monomers and dimers)
 - baryons (rep. by oriented self-avoiding loops)
- and chiral symmetry breaking/restoration:

 $\mathsf{U}_{\mathsf{A}}(1): \qquad \chi(x) \mapsto e^{i\eta_5(x)\theta_{\mathsf{A}}}\chi(x), \ \bar{\chi}(x) \mapsto \bar{\chi}(x)e^{i\eta_5(x)\theta_{\mathsf{A}}}, \qquad \eta_5(x)$

$$\Sigma_{5}(x) = (-1)^{\sum_{\nu=0}^{d} x_{\nu}}$$

is spontaneously broken below T_c ,

hence its phase diagram might be similar to the QCD phase diagram

SC-LQCD as effective theory for nuclear matter:

- derive nuclear interactions between hadrons from (Lattice) QCD
- transition at high density is the nuclear transition

Just another effective model for QCD?

• yes and no: think of SC-LQCD rather as a 1-parameter deformation of QCD

SC-QCD Partition Function (1)

Partition function for $SU(N_c)$:

$$\mathcal{Z} = \int \prod_{x} d\bar{\chi} d\chi e^{2am_{q}M(x)} \prod_{\mu} \Big\{ \sum_{k_{\mu}(x)=0}^{N_{c}} \frac{(N_{c} - k_{\mu}(x))!}{N_{c}!k_{\mu}(x)!} (M(x)M(x+\hat{\mu}))^{k_{\mu}(x)} \Big\}$$

$$+ \kappa \left(\rho(x,y)^{N_{\rm c}} \bar{B}(x) B(x+\hat{\mu}) + (-\rho(y,x))^{N_{\rm c}} \bar{B}(x+\hat{\mu}) B(x) \right) \right\}$$



SC-QCD Partition Function (1)

Partition function for $SU(N_c)$:

$$\begin{aligned} \mathcal{Z} &= \int \prod_{x} d\bar{\chi} d\chi e^{2am_{q}M(x)} \prod_{\mu} \Big\{ \sum_{k_{\mu}(x)=0}^{N_{c}} \frac{(N_{c} - k_{\mu}(x))!}{N_{c}!k_{\mu}(x)!} \left(M(x)M(x + \hat{\mu}) \right)^{k_{\mu}(x)} \\ &+ \kappa \left(\rho(x, y)^{N_{c}} \bar{B}(x)B(x + \hat{\mu}) + (-\rho(y, x))^{N_{c}} \bar{B}(x + \hat{\mu})B(x) \right) \Big\} \end{aligned}$$

Only confined, colorless degrees of freedom remain after link integration ($N_c = 3$):

• Mesons $M(x) = \overline{\chi}(x)\chi(x)$, represented by monomers and dimers (non-oriented meson hoppings):

• Baryons
$$B(x) = \frac{1}{3!} \epsilon_{i_1 \dots i_3} \chi_{i_1}(x) \dots \chi_{i_3}(x)$$

form self-avoiding oriented loops:

$$\rho(x, y) = \eta_{\hat{\mu}}(x) \exp(\pm a_{\tau} \mu) \delta_{\hat{\mu}\hat{0}}$$

 $\textit{n(x)} \in \{0, 1, \ldots, 3\}$

$$k_{\mu}(x) \in \{0,1,\ldots,3\}$$

 $\bar{B}(x)B(y)\in\{0,1\}$

 Note: baryons transform under gauge trafo Ω ∈ U(3) as B(x) → B(x) det Ω
 ⇒ not gauge invariant, only SU(3) contains baryons (κ = 1), U(3) purely mesonic (κ = 0)

SC-QCD Partition Function (2)

Exact rewriting of SC-QCD partition function (no approximation!):

$$\mathcal{Z}(m_q, \mu, N_{\tau}) = \sum_{\{k,n,l\}} \prod_{b=(x,\hat{\mu})} \frac{(3-k_b)!}{3!k_b!} \prod_x \frac{3!}{n_x!} (2am_q)^{n_x} \prod_l w(\ell, \mu)$$

• Grassmann constraint:

color neutral states at each site

$$n_x + \sum_{\hat{\mu}=\pm \hat{0},\ldots \pm \hat{d}} k_{\hat{\mu}} = 3 \qquad \forall x \in N_\sigma^{-3} \times N_\tau$$

• weight for baryon loop I (sign $\sigma(\ell)$):

$$w(\ell,\mu) = \frac{1}{\prod_{x \in \ell} 3!} \sigma(\ell) e^{3N_{\tau} r_l a_{\tau} \mu}$$

• in the following: restrict to chiral limit, where monomer density $\langle n \rangle = 0$



SC-LQCD at finite temperature

How to vary the temperature?

- $aT = 1/N_{\tau}$ is discrete with N_{τ} even
- $aT_c \simeq 1.5$ \Rightarrow we cannot address the phase transition!

Solution: introduce an **anisotropy** γ in the Dirac couplings:

$$\mathcal{L}_{ ext{QCD}} = \sum_{\mu} rac{\gamma^{\delta_{\mu 0}}}{2} \eta_{
u}(x) \left(e^{\mu \delta_{\mu 0}} ar{\chi}(x) U_{
u}(x) \chi(x+\hat{\mu}) - e^{-\mu \delta_{\mu 0}} ar{\chi}(x+\hat{\mu}) U^{\dagger}_{\mu}(x) \chi(x)
ight)$$

Should we expect $a/a_{\tau} = \gamma$, as suggested at weak coupling?

• No: meanfield predicts $a/a_{\tau} = \gamma^2$, since $\gamma_c^2 = N_{\tau} \frac{(d-1)(N_c+1)(N_c+2)}{6(N_c+3)}$

 \Rightarrow sensible, N_{τ} -independent definition of the temperature:

$$aT\simeq rac{\gamma^2}{N_ au}$$

• Moreover: SC-QCD partition function is a function of γ^2 :

$$\mathcal{Z}(m_{q},\mu,\gamma,N_{\tau}) = \sum_{\{k,n,l\}} \prod_{b=(x,\mu)} \frac{(3-k_{b})!}{3!k_{b}!} \gamma^{2k_{b}\delta_{\mu 0}} \prod_{x} \frac{3!}{n_{x}!} (2am_{q})^{n_{x}} \prod_{l} w(\ell,\mu)$$

However: precise correspondence between a/a_{τ} and γ^2 not known

SC-LQCD at finite Temperature and Continuous Time:



$$N_ au o \infty, \qquad \gamma o \infty, \qquad \gamma^2/N_ au$$
 fixed

• same as in analytic studies: $a_{\tau} = 0$, $aT = \beta^{-1} \in \mathbb{R}$



SC-LQCD at finite Temperature and Continuous Time:

Strategy for unambiguous answer: the continuous Euclidean time limit (CT-limit):

$$N_{ au} o \infty, \qquad \gamma o \infty, \qquad \gamma^2/N_{ au} \quad {
m fixed}$$

$$ullet$$
 same as in analytic studies: $a_ au=$ 0, $a\mathcal{T}=eta^{-1}\in\mathbb{R}$

Several advantages of continuous Euclidean time approach:

- ambiguities arising from the functional dependence of observables on the anisotropy parameter will be circumvented, only one parameter setting the temperature
- ullet no need to perform the continuum extrapolation $N_ au o \infty$
- allows to estimate critical temperatures more precisely, with a faster algorithm (about 10 times faster than $N_t = 16$ at T_c)
- baryons become static in the CT-limit, the sign problem is completely absent!

Origin of Continuous Time / Diagrammatic Monte Carlo

Continuous time (CT) methods were introduced in Quantum Monte Carlo: Suzuki-Trotter decomposition $\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2$ allows mapping onto classical spin system and sampling of diagrammatic expansion in continuous time

First proposed for the Heisenberg quantum antiferromagnet (Beard & Wiese, 1996):

 persue a world-line formulation
 (i. e. rewrite the partition function in terms of transition/decay probabilities)



Phys. Rev. Lett. 77 (1996) 5132



Origin of Continuous Time / Diagrammatic Monte Carlo

Continuous time (CT) methods were introduced in Quantum Monte Carlo: Suzuki-Trotter decomposition $\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2$ allows mapping onto classical spin system and sampling of diagrammatic expansion in continuous time

First proposed for the Heisenberg quantum antiferromagnet (Beard & Wiese, 1996):

- persue a world-line formulation (i. e. rewrite the partition function in terms of transition/decay probabilities)
- 2

make time direction continuous, transitions may occur at any time



Phys. Rev. Lett. 77 (1996) 5132



Origin of Continuous Time / Diagrammatic Monte Carlo

Continuous time (CT) methods were introduced in Quantum Monte Carlo: Suzuki-Trotter decomposition $\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2$ allows mapping onto classical spin system and sampling of diagrammatic expansion in continuous time

First proposed for the Heisenberg quantum antiferromagnet (Beard & Wiese, 1996):

persue a world-line formulation (i. e. rewrite the partition function in terms of transition/decay probabilities)



make time direction continuous, transitions may occur at any time



Situation today:

- rich literature for quantum impurity systems (see review by Gull *et al* 2010) based on diagrammatic Monte Carlo
- now: continuous time method applied to gauge theories

Continuous Time Partition Function (1)

In the following: restrict to chiral limit $m_q = 0$, where monomers are absent. Key observation: multiple spatial dimers are suppressed with powers of γ^{-2} :

- double/triple spatial dimers become resolved into single dimers as $a_{\tau} \simeq a/\gamma^2 \rightarrow 0$
- single spat. dimers survive (constant density)

• baryonic spat. hops are suppressed with γ^{-1}





Continuous Time Partition Function (1)

The partition function can be decomposed into spatial and temporal parts, i. e.:

- in spatial dimers (meson hoppings) and two types of temporal intervals in between: dashed (3-0-3-0-...) and solid intervals (2-1-2-1-...)
- the weight of a configuration only depends on the kind and number of vertices at which spatial hoppings are attached to solid/dashed lines:
 - "L"-vertices of weight $v_L = 1$, and
 - "T"-vertices of weight $v_T = 2/\sqrt{3}$, where a solid line emits a spatial dimer.
- n_L(x) and n_T(x) denote the number of T-vertices and L-vertices at spatial position x.





Continuous Time Partition Function (1)

Partition function in the limit of large
$$\gamma^2$$
, N_{τ} with $T = \gamma^2/N_{\tau}$:

$$\mathcal{Z}(\gamma, N_{\tau}) \simeq \gamma^{3V} \sum_{\{k, n_B(x)\}} \prod_{x \in V_B} e^{3n_B(x)\mu/T} \prod_{x \in V_M} \prod_{b=(x,\hat{i})} \frac{1}{3} \gamma^{-2k_b} \prod_{b_0=(x,\hat{0})} \frac{(3-k_{b_0})!}{3!k_{b_0}!}$$

$$= \sum_{\{k, n_B(x)\}} e^{3n_B\mu/T} \prod_{x \in V_M} \left(\frac{v_L}{\gamma}\right)^{n_L(x)} \left(\frac{v_T}{\gamma}\right)^{n_T(x)}, \quad n_B(x) \in \{-1, 0, 1\}$$

with $V_M \dot{\cup} V_B = N_\sigma^{\ 3}$ the mesonic/baryonic subvolumes and $n_B = \sum_x n_B(x)$ the baryon number

- typical 2-dimensional configurations in discrete and continuous time at the same temperature
- no multiple dimers, only static baryons in continuous time





Continuous Time Partition Function (3)

Final step: partition function in $\beta = 1/aT$:

- expansion in powers of γ^{-2} , i. e. in total number of spatial hoppings: $\kappa = \frac{1}{2} \sum_{x \in V_{**}} (n_L(x) + n_T(x))$
- sum over all spatial hopping positions $\sim N_{ au}/2$
 - \Rightarrow expansion in inverse temperature $\beta \simeq N_{\tau}/\gamma^2$:

$$\mathcal{Z}(\beta) = \sum_{\kappa \in 2\mathbb{N}} \frac{(\beta/2)^{\kappa}}{\kappa!} \sum_{\mathcal{C} \in \Gamma_{\kappa}} v_T^{n_T(\mathcal{C})} e^{\beta 3\mu B(\mathcal{C})}, \quad n_T = \sum_x n_T(x)$$

- Γ_{κ} is the set of equivalence classes of configurations with κ spatial hoppings
- $C \in \Gamma_{\kappa}$ is a representative of all configurations obtained from shifts of spatial hoppings which leave their time ordering unchanged
- prefactor is weight for equivalence class of time ordered graph $C \in \Gamma_{\kappa}$ (weight does not depend on specific time coordinates):

$$\frac{1}{2^{\kappa}} \int_0^\beta dk_1 \int_{k_1}^\beta dk_2 \dots \int_{k_{\kappa-1}}^\beta dk_{\kappa} v_T^{n_T(\mathcal{C})} = \frac{1}{\kappa!} \left(\frac{\beta}{2}\right)^{\kappa} v_T^{n_T(\mathcal{C})}$$

Continuous Time Partition Function (3)

Final step: partition function in $\beta = 1/aT$:

- expansion in powers of γ^{-2} , i. e. in total number of spatial hoppings: $\kappa = \frac{1}{2} \sum_{x \in V_{**}} (n_L(x) + n_T(x))$
- ullet sum over all spatial hopping positions $\sim N_{ au}/2$
 - \Rightarrow expansion in inverse temperature $\beta \simeq N_{\tau}/\gamma^2$:

$$\mathcal{Z}(\beta) = \sum_{\kappa \in 2\mathbb{N}} \frac{(\beta/2)^{\kappa}}{\kappa!} \sum_{\mathcal{C} \in \Gamma_{\kappa}} v_T^{n_T(\mathcal{C})} e^{\beta 3\mu B(\mathcal{C})}, \quad n_T = \sum_x n_T(x)$$

Combinatorics governed by constraints concerning assignments of emission/absorption event to vertices:

• state vector χ characterizing time slice, $\chi(t) = (\chi_1, \dots \chi_V)$, $\chi_x \in \{|0\rangle, \dots |N_c\rangle\}$

• spatial dimers acts at time t_i on $\chi(t)$: $D_{\langle x,y\rangle} = (J_x^{\pi(x)}J_t^{\pi(y)})$ with (for $N_c = 3$) $J^+ = \begin{pmatrix} 0 & & \\ v_L & 0 & & \\ & v_T & 0 & \\ & & v_L & 0 \end{pmatrix}$, $J^- = (J^+)^T$ and $\pi(x) = \pm 1$ the parity of site x

• peridicity implies: $M\chi(0) = \chi(\beta) \equiv \chi(0)$, i. e. $M = \prod_{i=1}^{\kappa} D_{<x,y>} t_i \equiv \mathbb{1}$

• and the "Grassmann constraint" is: $J^+|N_{\rm c}
angle=0,~J^-|0
angle=0$ (forbidden)

Continuous Time Partition Function (3)

Final step: partition function in $\beta = 1/aT$:

- expansion in powers of γ^{-2} , i. e. in total number of spatial hoppings: $\kappa = \frac{1}{2} \sum_{x \in V_{el}} (n_L(x) + n_T(x))$
- ullet sum over all spatial hopping positions $\sim N_{ au}/2$
 - \Rightarrow expansion in inverse temperature $\beta \simeq N_{\tau}/\gamma^2$:

$$\mathcal{Z}(\beta) = \sum_{\kappa \in 2\mathbb{N}} \frac{(\beta/2)^{\kappa}}{\kappa!} \sum_{\mathcal{C} \in \Gamma_{\kappa}} v_T^{n_T(\mathcal{C})} e^{\beta 3\mu B(\mathcal{C})}, \quad n_T = \sum_x n_T(x)$$

successfully used so far: Worm algorithm in continuous time here: attempt diagrammatic MC based on the diagrammatic expansion in κ



Short Comment on CT-Worm Algorithm

CT Worm algorithm is derived from directed path Worm algorithm (Adams & Chandrasekharan, 2003):

- key step: hopping times are uniformly distributed and according to the statistics of a Poisson process:
- the dashed/solid interval lengths are exponentially distributed:

$$P(\Delta\beta) = e^{-\lambda\Delta\beta}, \quad \Delta\beta \in [0, \beta = 1/aT]$$

λ is the "decay constant" for spatial dimer emissions:



$$\lambda = d_M(x)/4, \qquad d_M(x) = 2d - \sum_{\hat{\mu}=\pm i} |n_B(x+\hat{\mu})|$$

with $d_M(x)$ the number of mesonic neighbors at x

• idea of continuous time worm in SC-QCD: use probability distribution $p(\Delta\beta)$ for spatial dimer emission after time interval $\Delta\beta$

Generalization to arbitrary $SU(N_c)$

Continuous time methods can be applied to any gauge group $SU(N_c)$:

- baryons only become static for $SU(N_c)$ with $N_c \ge 3$
- N_c = 2: diquark loops can have spatial hoppings, no T-vertices present
- large $N_{\rm c}$ feasible





- list of line types: dashed, single, double, triple...
- for N_c > 3: generalization of T-vertices change line-type by one unit or its parity

Crosscheck with analytic results for U(1)

Analytic solution of the U(1) system on $2 \times N_{\tau}$ latties:

$$\chi(N_{\tau},\gamma^{2}) = \frac{1}{2} \tanh\left(\frac{N_{\tau}}{2}\operatorname{acsch}(\gamma^{2})\right) \left((1+\gamma^{-4})^{-\frac{1}{2}} + \tanh\left(\frac{N_{\tau}}{2}\operatorname{acsch}(\gamma^{2})\right)\right)$$
$$\chi(T) = \frac{1}{2} \tanh\left(1/2T\right) \left(1 + \tanh\left(1/2T\right)\right)$$



Wolfgang Unger, ETH Zürich

DMC for SC-LQCD

SC-QCD Phase Diagram

Studied via CT-Worm algorithm: arXiv:1111.1434 [hep-lat] Comparison of phase diagram with $N_{\tau} = 4$ data (M. Fromm, 2010):

• CT-data compared to $N_{ au} = 4$ data for identification

 $\pmb{a}\mu=\gamma^2\pmb{a}_{ au}\mu$

- $\bullet\,$ behavior at low μ agrees well, location of TCP agrees within errors
- no re-entrance is seen at small temperatures



What is Diagrammatic Monte Carlo?

Importance sampling of diagrams described in terms of a perturbative series:

- each term in the diagrammatic expansion of the partition function is represented by a world line configuration
- perturbative series may not converge, but at any finite volume and temperature, only a finite number of orders contribute
- CT-Worm is one of the DMC techniqes, others are the loop cluster algorithm (Evertz et al.), stochastic series expansion (Sandvik)

Here: make use of insertions/shifts of world line decorations:

- Problem: vanishing acceptance rate: $p = (t\delta\tau)^2 \rightarrow 0 \Rightarrow p_{ins} = min(1, p) \rightarrow 0$
- Solution: integrate over all possible insertions within interval Λ : $p = \int_0^{\Lambda} d\tau_1 \int_{\tau_1}^{\Lambda} d\tau_2 t^2 = \frac{\Lambda^2 t^2}{2} \neq 0 \quad \Rightarrow p_{\text{ins}} = \min(1, p) \neq 0$

Motivation: Generalization of SC-QCD to 2 chiral flavors!

Aim: obtain phase diagram for 2-flavor SC-QCD, where **pion exchange** may play a crucial role for nuclear transition

- but: at present, no 2-flavor formulation for staggered SC-QCD suitable for MC present
- already the mesonic sector has a severe (unphysical) sign problem in dimer representation
- 2 new types of flavored dimers give negative sign in mesonic loops already for U(2).

Observation in continuous time formulation:

- flux representation for 2 different flavors can be composed such that cancellations appear
- first step in this direction: Monte Carlo for insertion/removal of rectangles rather than worm algorithm



Diagrammatic Monte Carlo

The Hopping parameter Expansio

Diagrammatic expansion for SC-QCD amounts to hopping parameter expansion in $\beta/2$ on N_s^3 with time ordering of L- and T-vertices:

- label spatial dimers with time index *i* = 1,...κ and attach at its ends vertices with weight v_L, v_T
- enumeration of Γ_κ, i. e. all valid configurations consistent with parity (e. g. even/odd interval lengths, in sketch: even intervals between L- and T-vertices highlighted) not feasible



Wolfgang Unger, ETH Zürich

Diagrammatic Monte Carlo

The Hopping parameter Expansion of CT-SC-QCD



- label spatial dimers with time index *i* = 1,...κ and attach at its ends vertices with weight v_L, v_T
- enumeration of Γ_κ, i. e. all valid configurations consistent with parity (e. g. even/odd interval lengths, in sketch: even intervals between L- and T-vertices highlighted) not feasible

Data structure used in DMC for sampling Γ_{κ} : • state vector $\chi(x, t = 0) \in \{0, \dots, N_c\}$

• set of time ordered spatial dimers $\{\langle x_1^{V_1}, y_1^{W_1} \rangle, \langle x_2^{V_2}, y_2^{W_2} \rangle, \dots \langle x_{\kappa}^{V_{\kappa}}, y_{\kappa}^{W_{\kappa}} \rangle\}$ with $V_i, W_i \in \{L, T\}$

Some time-ordered diagrams of order $\kappa=4{:}$



Flux Representation

Combinatorics of diagrams in Γ_{κ} goverened by assignment of

- emission/absorption events to vertices, or
- equivalently: even/odd lengths of time intervals

Observation: emission-absorption ordering induces orientation on rectangles:

- spatial dimers have orientation from emission to absorption site
- solid lines can be consistently oriented (colors for illustration)
- 2-dim. SC-QCD partition function can be conceived as composed of static lines and oriented rectangles



re-expressing a 2-dim. configuration in terms of oriented rectangles and oriented static lines

Algorithmic Details (1)

Apply Metropolis-Hastings Alogrithm to SC-QED:

• configuration with κ spatial dimers has weight $w(C^{(\kappa)}) = \frac{1}{\kappa!} \left(\frac{\beta}{2}\right)^{\kappa}$, κ always even

• insertion:
$$p_{\text{ins}}\left(C_1^{(\kappa)} \to C_2^{(\kappa+2)}\right) = \min\left[1, \frac{\mathrm{w}(\mathrm{C}_2^{(\kappa+2)})}{\mathrm{w}(\mathrm{C}_1^{(\kappa)})} \frac{\mathrm{A}_{\text{rem}}(\mathrm{C}_2^{(\kappa+2)} \to \mathrm{C}_1^{(\kappa)})}{\mathrm{A}_{\text{ins}}(\mathrm{C}_1^{(\kappa)} \to \mathrm{C}_2^{(\kappa+2)})}\right]$$

• removal:
$$p_{\text{rem}}\left(C_1^{(\kappa)} \to C_2^{(\kappa-2)}\right) = \min\left[1, \frac{\mathrm{w}(\mathrm{C}_2^{(\kappa-2)})}{\mathrm{w}(\mathrm{C}_1^{(\kappa)})} \frac{\mathrm{A}_{\text{ins}}(\mathrm{C}_2^{(\kappa-2)} \to \mathrm{C}_1^{(\kappa)})}{\mathrm{A}_{\text{rem}}(\mathrm{C}_1^{(\kappa)} \to \mathrm{C}_2^{(\kappa-2)})}\right]$$

- proposal probabilities $A_{ins}(C_1 \rightarrow C_2)$, $A_{rem}(C_2 \rightarrow C_1)$ not independent of C_1 , C_2 , need to be calculated for each update in an efficient way
- proposal probabilities depend on the way how insertion, removal is proposed
- several options how to implement rectangle updates, here: split into two parts, insertion/removal of pair (easy part, local), moving them apart (shift update difficult part, non-local)

Algorithmic Details (2)

Apply Metropolis-Hastings Alogrithm to SC-QED:

- insertion update: $\kappa \mapsto \kappa + 2$:
 - choose a specific insertion for $\ensuremath{\mathcal{C}}_1$
 - determine number n_p^{ins} of possible insertions (cheap: at each bond and t_i insertion is possible if parity agrees)
 - determine number of distinct insertions n_c^{ins} which would gives the same new config. C_2

$$\Rightarrow A_{\rm ins}(C_1 \to C_2) = n_c^{\rm ins} / n_p^{\rm ins}$$

- determine number $n_p^{\rm rem}$ of possible removals in C_2 (cheap: computed along with possible insertions)
- determine number of distinct removals $n_c^{\rm rem}$ which would gives the same old config. ${\cal C}_1$

$$\Rightarrow \quad A_{\rm rem}(C_2 \to C_1) = n_c^{\rm rem}/n_p^{\rm rem}$$

 removal update: κ → κ − 2: similar to the above

DMC flow chart:

insertion and removal updates for pairs of oppositely oriented spatial dimers



Algorithmic Details (2)

Apply Metropolis-Hastings Alogrithm to SC-QED:

- static line update: change
 k₀(x) → k₀(x) ± 1, if consitent
 with vertices on site x
- shift update: needed for ergodicity, and in simplified insertion/removal (only pairs): essential!
 - $A_{\rm shift}$ trivial, but shifts may involve large number of flow inversions
 - need to construct clusters which spatial dimers are affected
 - demanding in eihter memory or CPU time

DMC flow chart: insertion and removal updates for pairs

of oppositely oriented spatial dimers



Wolfgang Unger, ETH Zürich

Preliminary Results

So far: only spatial dimer measurements in 1 spatial dimension possible

- First measurement: comparing CT-Worm with DMC
- specific heat (can be obtained from spatial dimers) for U(1) (left) and U(3) (right) on 1+1-dimensional lattice:



 observation: DMC performs better at small volumes, but not so well on large volumes (improvements on shift update?)

• also DMC becomes demanding in memory for large volumes (for shift updates)

Wolfgang Unger, ETH Zürich

DMC for SC-LQCD

Diagrammatic Monte Carlo

Generalization to higher dimensions:

- so far: every graph composed of only planar rectangles
- in spatial dimensions d > 1, algorithm is not ergodic

Flip update:

- $\bullet\,$ does not change order in $\beta\,$
- but might add/remove T-vertices → another Metropolis update . . .
- sufficient to produce any higher-dimensional closed loops occuring in hopping parameter expansion



DMC for SC-LQCD



Prospects:

- CT partition function: new formulation for analytic treatment
- hope: extend formulation for two flavors (incorporates pion exchange)
- $\bullet\,$ extension to SU(3) with finite baryon chem. potential straight forward Drawbacks
 - generalization to higher dimensions turns out to be very difficult
 - not yet possible to study periodic boundary conditions
 - in contrast to worm: no 2-point function for free (but: cluster-size as a measure for susceptibility?)
 - might turn out that worm algorithm is more efficient at large volumes

Backup Slides

Why Study Strong Coupling QCD on the Lattice?

Two possible scenarios for the relation between SC-LQCD (back) and the (L)QCD phase diagram for four flavors (front):

