Diagrammatic Monte Carlo simulations of staggered fermions at finite coupling

Hélvio Vairinhos

ETH zürich

with Philippe de Forcrand

JHEP 12 (2014) 038

+ *in preparation*

Kobe, Japan
16 Jul 2015

Motivation

To determine the phase diagram of nuclear matter at finite temperature T and baryon chemical potential μ_B from first principles.

$$Z = \int [\mathcal{D}\chi \mathcal{D}\bar{\chi} \mathcal{D}U] \, e^{-S_g(U) + \bar{\chi} \not{D}(\mu, m) \chi} = \int [\mathcal{D}U] \, e^{-S_g(U)} \det(\not{D}(\mu, m))$$

- **Sign problem:** $\det(\not{D}(\mu, m))$ is complex-valued, in general, hence it cannot have a probabilistic interpretation.
- **Our approach:** Gauge integration before Grassmann integration.
- **Why?**
  1. The sign problem is representation-dependent: in the basis of eigenstates $|\Psi_i\rangle$ of the QCD Hamiltonian, the sign problem does not exist, by definition:

     $$Z = \mathrm{Tr}\Big\{e^{-\beta \hat{H}}\Big\} = \mathrm{Tr}\Big\{e^{-\frac{\beta}{N}\hat{H}} \sum_i |\Psi_i\rangle\langle\Psi_i| e^{-\frac{\beta}{N}\hat{H}} \sum_j |\Psi_j\rangle\langle\Psi_j| \cdots \Big\}$$

     for which $\langle\Psi_i| e^{-\beta \hat{H}} |\Psi_j\rangle \geq 0, \ \forall i, j$.
  2. *A priori* gauge integration yields an ensemble color-neutral fermionic states, arguably closer to the asymptotic eigenstates of QCD (due to confinement).

Motivation

To determine the phase diagram of nuclear matter at finite temperature T and baryon chemical potential μ_B from first principles.

$$Z = \int [\mathcal{D}\chi \mathcal{D}\bar{\chi} \mathcal{D}U] \, e^{-S_g(U) + \bar{\chi} \not{D}(\mu,m)\chi} = \int [\mathcal{D}U] \, e^{-S_g(U)} \det(\not{D}(\mu, m))$$

- **Sign problem:** $\det(\not{D}(\mu, m))$ is complex-valued, in general, hence it cannot have a probabilistic interpretation.
- **Our approach:** Gauge integration before Grassmann integration.
- **Goal:** Construct and simulate link-less representations of lattice gauge theories with staggered fermions at a finite chemical potential:
  1. Compact lattice QED, $N_f = 1$ ✓ (today)
  2. Compact lattice QED, $N_f > 1$ ✗ (for the future)
  3. $SU(2)$ gauge theory, $N_f \geq 1$ ✗ (for the future)
  4. $SU(3)$ gauge theory, $N_f \geq 1$ ✗ (for the future)

Integrating out the gauge fields

- Integrating out the link variables directly: only possible for $\beta = 0$

$$Z = \int [\mathcal{D}\chi\mathcal{D}\bar{\chi}\mathcal{D}U] \prod_{x,\mu} e^{\eta_{x\mu}\mathrm{Tr}\{\bar{\chi}_x U_{x\mu}\chi_{x+\hat{\mu}} - \bar{\chi}_{x+\hat{\mu}} U^\dagger_{x\mu}\chi_x\}} \prod_x e^{2am\bar{\chi}_x\chi_x}$$

$$= \sum_{\{n,k,C\}} \left(\prod_x \frac{N!}{n_x!}(2am)^{n_x} \right) \left(\prod_{x,\mu} \frac{(N-k_{x\mu})!}{N!k_{x\mu}!} \right) \left(\frac{1}{N!^{|C|}} \underbrace{\sigma(C)}_{\pm 1} \right)$$

Rossi & Wolff '84, Karsch & Mütter '89

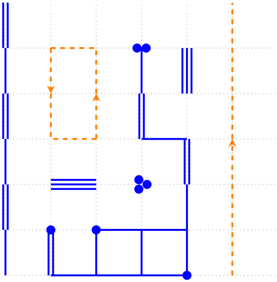
Degrees of freedom: monomers, dimers, loops

x ●	$(\bar{\chi}_x\chi_x)^{n_x}$	$n_x \in \{0,\ldots,N\}$
x ━━ y	$(\bar{\chi}_x\chi_x\bar{\chi}_y\chi_y)^{k_{xy}}$	$k_{xy} \in \{0,\ldots,N\}$
x - -➤- - y	$(\bar{B}_y B_x)^{b_{xy}}$	$b_{xy} \in \{0,1\}$
x - -◀- - y	$(\bar{B}_x B_y)^{\bar{b}_{xy}}$	$\bar{b}_{xy} \in \{0,1\}$

Grassmann constraints:

$$n_x + \sum_{\pm\mu}(k_{x\mu} + Nb_{x\mu}) = n_x + \sum_{\pm\mu}(k_{x\mu} + N\bar{b}_{x\mu}) = N$$

Admissible $SU(3)$ state:

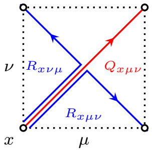


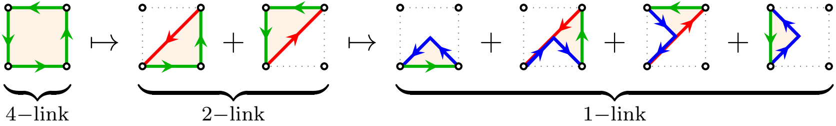
- Integrating out the link variables directly: only possible for $\beta = 0$
- Introduce free auxiliary plaquette variables: $Q_{x\mu\nu}, R_{x\mu\nu}$ HV & de Forcrand '14

$$Z = \int [\mathcal{D}U] \prod_p e^{\frac{\beta}{N}\mathrm{ReTr}(U_p)} = \int \mathcal{G}_\beta[Q,R] \prod_{x,\mu} \int dU\, e^{\frac{\beta}{N}\mathrm{ReTr}(J^\dagger_{x\mu}U)}$$

$$\mathcal{G}_\beta[Q,R] = [\mathcal{D}Q\mathcal{D}R]\, e^{-\frac{3\beta}{2N}\mathrm{Tr}(QQ^\dagger)} e^{-\frac{\beta}{2N}\mathrm{Tr}(RR^\dagger)}$$

$$J_{x\mu} = \sum_{\nu\neq\mu} (R^\dagger_{x-\hat{\nu},\nu\mu} Q_{x-\hat{\nu},\nu\mu} + R_{x\mu\nu})$$





- **Advantages:**
  - Exact linearization of the Wilson plaquette action.
  - Straightforward generalization for staggered flavours: $\frac{\beta}{2N} J_{x\mu} + \eta_{x\mu}\chi^\alpha_x \bar{\chi}^\alpha_{x+\mu}$
- **Disadvantages:** greater complexity, larger autocorrelations...

Bosonic variables $Q_{x\mu\nu}, R_{x\mu\nu} \in \mathbb{C}$ decouple the 4 links around the plaquette, reducing the Boltzmann factor to a product of solvable $U(1)$ **one-link integrals**:

$$\int_{U(1)} dU\, e^{\beta \mathrm{Re}(J^\dagger U)} = I_0(\beta|J|)$$

$\Rightarrow$ 0-link representation of the **partition function** of compact $U(1)$ lattice gauge theory:

$$Z = \int [dU] \prod_p e^{\beta \mathrm{Re}(U_p)} = \int \mathcal{G}_\beta[Q,R] \prod_{x,\mu} I_0(\beta|J_{x\mu}|)$$

Loop observables in the 0-link representation,

$$\langle W(C) \rangle = \left\langle \mathrm{Tr} \prod_{l \in C} U_l \right\rangle = \left\langle \mathrm{Tr} \prod_{l \in C} \mathcal{U}_l \right\rangle$$

are defined in terms of **effective links**:

$$\mathcal{U}_l = \langle U \rangle_{J_l} = \int dU\, U\, e^{\beta \mathrm{Re}(J_l^\dagger U)} = \frac{I_1(\beta|J_l|)}{I_0(\beta|J_l|)} \frac{J_l}{|J_l|}$$

The 0-link representation of the **partition function** of $N_f = 1$ compact lattice QED is easy to obtain:

$$\begin{aligned} Z(\beta, m) &= \int [dU] \prod_p e^{\beta \mathrm{Re}(U_p)} \prod_{x,\mu} e^{\bar{\chi}_x U_{x\mu} \chi_{x+\hat{\mu}} - \bar{\chi}_{x+\hat{\mu}} U^\dagger_{x\mu} \chi_x} \prod_x e^{2am\bar{\chi}_x \chi_x} \\ &= \int \mathcal{G}_\beta[Q, R] \prod_x I_0(\beta |J_{x\mu}|) \sum_{\{n,k,C\}} \sigma(C) \prod_x (2am)^{n_x} \prod_{i=1}^{\#C} 2\mathrm{Re}(\mathcal{U}(C_i)) \end{aligned}$$

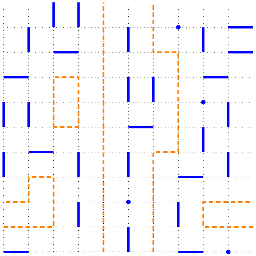
Degrees of freedom: monomers, dimers, loops

x ●	$(\bar{\chi}_x \chi_x)^{n_x}$	$n_x \in \{0, 1\}$
x ━━ y	$(\bar{\chi}_x \chi_x \bar{\chi}_y \chi_y)^{k_{xy}}$	$k_{xy} \in \{0, 1\}$
x - -➤- - y	$(\bar{\chi}_y \chi_x)^{b_{xy}}$	$b_{xy} \in \{0, 1\}$
x - -◄- - y	$(\bar{\chi}_x \chi_y)^{\bar{b}_{xy}}$	$\bar{b}_{xy} \in \{0, 1\}$

Grassmann constraints:

$$n_x + \sum_{\pm\mu} (k_{x\mu} + b_{x\mu}) = n_x + \sum_{\pm\mu} (k_{x\mu} + \bar{b}_{x\mu}) = 1$$

Admissible configuration:



Gauss's law: Only the zero (even) winding sector contributes

Simulating compact lattice QED

The bosonic d.o.f. (Q, R) and fermionic d.o.f. (n, k, C) are updated alternatingly:

- **Bosonic updates:**

  1. Local $U(1)$ heatbath wrt the one-link integral
  2. Local Gaussian heatbath of the auxiliary variables Q, R.
  3. Local Metropolis update, to correct for the (reweighted) electron loops.

$$\underbrace{\mathcal{G}_\beta[Q,R] \prod_{x,\mu} I_0(\beta|J_{x\mu}|)}_{\text{Heatbath}} \underbrace{\prod_{i=1}^{\#C} |2\mathrm{Re}(\mathcal{U}(C_i))|}_{\text{Metropolis}}$$

- **Fermionic updates:**

  Worm algorithms provide an efficient way to update constrained combinatorial system, e.g. monomer-dimer-loop configurations of compact lattice QED:

  1. "Meson" worm algorithm
  2. Electron worm algorithm

Prokof'ev & Svistunov '01

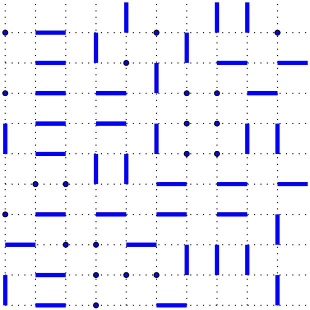
Adams & Chandrasekharan '03

Chandrasekharan & Jiang '06

"Meson" worm algorithm

Alternating sequence of active and passive updates along a worm path, which updates "mesonic" d.o.f., i.e. monomers and dimers at $\beta = 0$.

$$w = \prod_{x} (2am)^{n_x} \prod_{x,\mu} \xi_\mu^{2k_{x\mu}} \prod_{i=1}^{\#C} |2\mathrm{Re}(\mathcal{U}(C_i))|$$



Alternating sequence of **active** and **passive** updates along a worm path, which updates "mesonic" d.o.f., i.e. monomers and dimers at $\beta = 0$.

$$w = \prod_{x_a} (2am)^{n_{x_a}} \prod_{x_p} \left((2am)^{n_{x_p}} \prod_{\pm\mu} \xi_\mu^{2k_{x_p\mu}} \right) \prod_{i=1}^{\#C} |2\mathrm{Re}(\mathcal{U}(C_i))|$$

Active transitions:

$$\begin{cases} P_{ss}(x_a) = P_{\mu s}(x_a) = n_{x_a} \\ P_{s\nu}(x_a) = P_{\mu\nu}(x_a) = k_{x_a\mu} \end{cases}$$

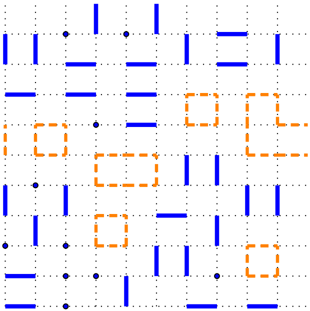
Passive transitions:

$$\begin{cases} P_{ss}(x_p) = P_{\mu s}(x_p) = \frac{(2am)^2}{(2am)^2 + \sum_\lambda \xi_\lambda^2 \, \delta_{\bar{C}}(x_p + \hat{\lambda})} \\ P_{s\nu}(x_p) = P_{\mu\nu}(x_p) = \frac{\xi_\nu^2 \, \delta_{\bar{C}}(x_p + \nu)}{(2am)^2 + \sum_\lambda \xi_\lambda^2 \, \delta_{\bar{C}}(x_p + \hat{\lambda})} \end{cases}$$

Electron worm algorithm

Alternating sequence of active and passive updates along a worm path, which updates dimers and electron loops at $\beta > 0$.

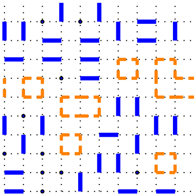
$$w = \prod_x (2am)^{n_x} \prod_{x,\mu} \xi_\mu^{2k_{x\mu}} \prod_{i=1}^{\#C} |2\mathrm{Re}(\mathcal{U}(C_i))|$$

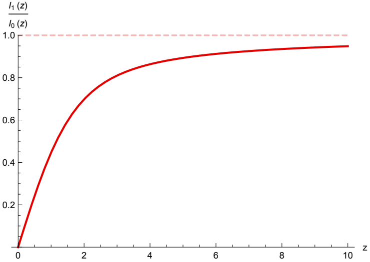


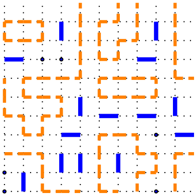
Alternating sequence of **active** and **passive** updates along a worm path, which updates dimers and electron loops at $\beta > 0$.

$$w = \prod_x (2am)^{n_x} \prod_{x_a} 1 \prod_{\pm\mu} \xi_\mu^{2k_{x_p\mu}+b_{x\mu}} \left(\frac{I_1(\beta|J_{x\mu}|)}{I_0(\beta|J_{x\mu}|)} \right)^{b_{x\mu}} \prod_{i=1}^{\#C} |2\cos(\vartheta(C_i))|$$

The ratio $\frac{I_1(\beta|J_{x\mu}|)}{I_0(\beta|J_{x\mu}|)}$ promotes deletion of loops at small β, and their creation at large β:





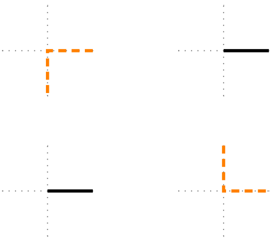


Electron worm algorithm

Alternating sequence of **active** and **passive** updates along a worm path, which updates dimers and electron loops at $\beta > 0$.

$$w = \prod_x (2am)^{n_x} \prod_{x_a} 1 \prod_{\pm\mu} \xi_\mu^{2k_{x_p\mu}+b_{x\mu}} \left(\frac{I_1(\beta|J_{x\mu}|)}{I_0(\beta|J_{x\mu}|)}\right)^{b_{x\mu}} \prod_{i=1}^{\#C} |2\cos(\vartheta(C_i))|$$

Active transitions:



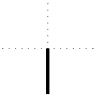
$$\begin{cases} P_{ss}(x_a) = n_x \\ P_{s\mu}(x_a) = \frac{2k_{x\mu}+|b_{x\mu}|}{2} \\ P_{\mu s}(x_a) = \frac{b_x}{2-2k_{x\mu}-|b_{x\mu}|} \\ P_{\mu\nu}(x_a) = \frac{2k_{x\mu}+|b_{x\mu}|}{2-2k_{x\mu}-|b_{x\mu}|} \end{cases}$$

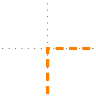
Electron worm algorithm

Alternating sequence of **active** and **passive** updates along a worm path, which updates dimers and electron loops at $\beta > 0$.

$$w = \prod_{x} (2am)^{n_x} \prod_{x_a} 1 \prod_{\pm\mu} \xi_{\mu}^{2k_{x_p\mu}+b_{x\mu}} \left(\frac{I_1(\beta|J_{x\mu}|)}{I_0(\beta|J_{x\mu}|)} \right)^{b_{x\mu}} \prod_{i=1}^{\#C} |2\cos(\vartheta(C_i))|$$

Passive transitions:



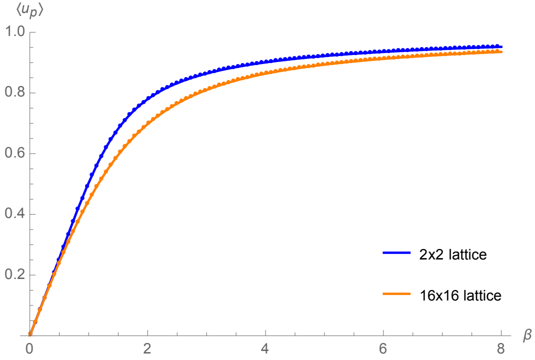


$$\begin{cases} P_{\mu\nu}(x_p) = \dfrac{\xi_\nu r_{1,x\nu}^{1-2q_{x\nu}} \left(1 - n_{x+\hat{\nu}}\right)}{\sum\limits_{\lambda\neq\nu} \xi_\lambda r_{1,x\lambda}^{1-2q_{x\lambda}} \left(1 - n_{x+\hat{\lambda}}\right) + \xi_\mu r_{1,x\mu}^{1-2(q_{x\mu}-1)}} \\[2ex] P_{\mu\mu}(x_p) = \dfrac{\xi_\mu r_{1,x\mu}^{1-2(q_{x\mu}-1)}}{\sum\limits_{\lambda\neq\nu} \xi_\lambda r_{1,x\lambda}^{1-2q_{x\lambda}} \left(1 - n_{x+\hat{\lambda}}\right) + \xi_\mu r_{1,x\mu}^{1-2(q_{x\mu}-1)}} \end{cases}$$

$$q_{x\mu} = 2k_{x\nu} + b_{x\nu} \qquad\qquad r_{x\mu} = \frac{I_1(\beta|J_{x\mu}|)}{I_0(\beta|J_{x\mu}|)}$$

Partition functions and vevs of loop operators are known exactly in the pure gauge sector for periodic $d = 2$ lattices, which only depend on the spacetime volume V and the area A enclosed by the loop operator,

$$Z_V(\beta) = \sum_n I_n^V(\beta) \qquad \langle W(C)\rangle = \frac{1}{Z_V(\beta)} \sum_n I_n^{V-A}(\beta) I_{n+1}^A(\beta)$$



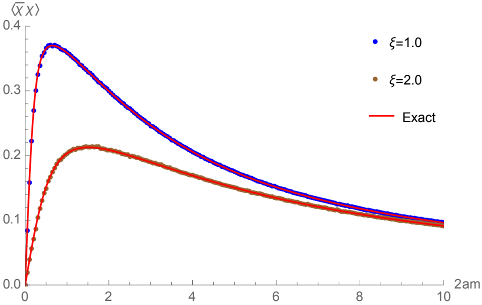
Consistency checks

Meson worm algorithm on a 4×4 lattice

Partition functions of compact lattice QED at $\beta = 0$ can be computed exactly in small $2d$ lattices, by enumerating perfect matchings in the excluded volume of monomer sites.

$$
\begin{aligned}
Z(\xi, m) \quad = \quad & 16\left(\xi^{16} + 4\xi^{12} + 7\xi^{8} + 4\xi^{4} + 1\right) + (2am)^{16} + 16\left(\xi^{2} + 1\right)(2am)^{14} + 8\left(13\xi^{4} + 24\xi^{2} + 13\right)(2am)^{12} \\
& + 32\left(\xi^{2} + 1\right)\left(11\xi^{4} + 17\xi^{2} + 11\right)(2am)^{10} + 8\left(83\xi^{8} + 256\xi^{6} + 354\xi^{4} + 256\xi^{2} + 83\right)(2am)^{8} \\
& + 64\left(11\xi^{10} + 37\xi^{8} + 63\xi^{6} + 63\xi^{4} + 37\xi^{2} + 11\right)(2am)^{6} \\
& + 32\left(13\xi^{12} + 40\xi^{10} + 81\xi^{8} + 96\xi^{6} + 81\xi^{4} + 40\xi^{2} + 13\right)(2am)^{4} \\
& + 64\left(\xi^{2} + 1\right)\left(2\xi^{12} + 2\xi^{10} + 8\xi^{8} + 5\xi^{6} + 8\xi^{4} + 2\xi^{2} + 2\right)(2am)^{2}
\end{aligned}
$$

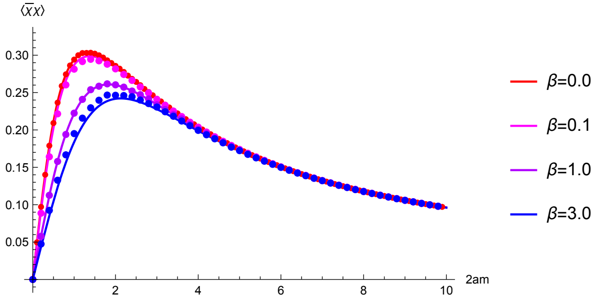
$$
a\langle\bar{\chi}\chi\rangle = \frac{1}{16}\frac{\partial \log Z(\xi, m)}{\partial(2am)}
$$



The partition function of compact lattice QED for any β and m can be computed exactly on a 2×2 lattice,

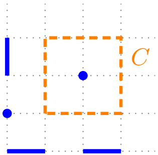
$$Z(\beta,m) = ((2am)^4 + 8(2am)^2 + 8)\sum_n I_n^4(\beta) + 8\sum_n I_n^3(\beta) I_{n+1}(\beta) + 4\sum_n I_n^2(\beta) I_{n+1}^2(\beta)$$

$$a\langle\bar{\chi}\chi\rangle = \frac{1}{Z(\beta,m)}(2am)((2am)^2+4)\sum_n I_n^4(\beta)$$



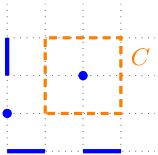
The **sign** s has a **fermionic** σ_F and a **bosonic** σ_B contribution:

$$s = \underbrace{(-1)^{N_-(C)+w_\tau(C)+1} \prod_{(x,\mu)\in C} \eta_{x\mu}}_{\sigma_F(C)} \times \underbrace{\mathrm{sign}\left(\prod_{i=1}^{\#C} 2\mathrm{Re}(\mathcal{U}(C_i))\right)}_{\sigma_B(C)}$$



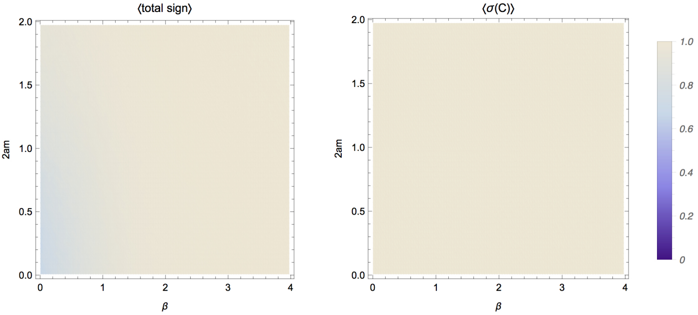
The **sign** s has a **fermionic** σ_F and a **bosonic** σ_B contribution:

$$s = \underbrace{(-1)^{N_-(C)+w_\tau(C)+1} \prod_{(x,\mu)\in C} \eta_{x\mu}}_{\sigma_F(C)} \times \underbrace{\text{sign}\left(\prod_{i=1}^{\#C} 2\text{Re}(\mathcal{U}(C_i))\right)}_{\sigma_B(C)}$$



which behave very differently...

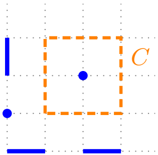
2×2 **lattice**



Sign problem
on a 4×4 lattice

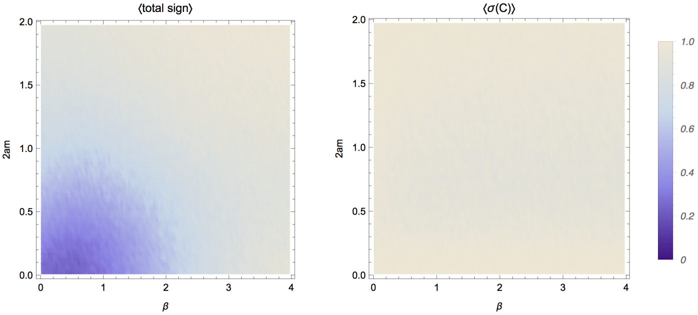
The **sign** s has a **fermionic** σ_F and a **bosonic** σ_B contribution:

$$s = \underbrace{(-1)^{N_-(C)+w_\tau(C)+1} \prod_{(x,\mu)\in C} \eta_{x\mu}}_{\sigma_F(C)} \times \underbrace{\mathrm{sign}\left(\prod_{i=1}^{\#C} 2\mathrm{Re}(\mathcal{U}(C_i))\right)}_{\sigma_B(C)}$$



which behave very differently...

4×4 **lattice**

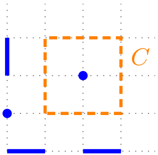


Sign problem

on a 6×6 lattice

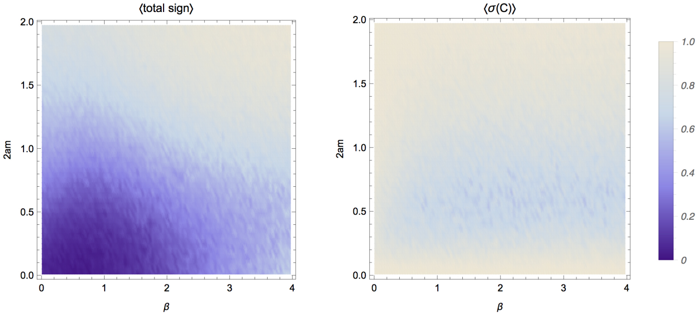
The **sign** s has a **fermionic** σ_F and a **bosonic** σ_B contribution:

$$s = \underbrace{(-1)^{N_-(C)+w_\tau(C)+1} \prod_{(x,\mu)\in C} \eta_{x\mu}}_{\sigma_F(C)} \times \underbrace{\operatorname{sign}\left(\prod_{i=1}^{\#C} 2\mathrm{Re}(\mathcal{U}(C_i))\right)}_{\sigma_B(C)}$$



which behave very differently...

6×6 **lattice**

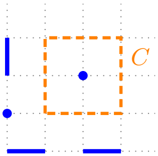


Sign problem

on a 8×8 lattice

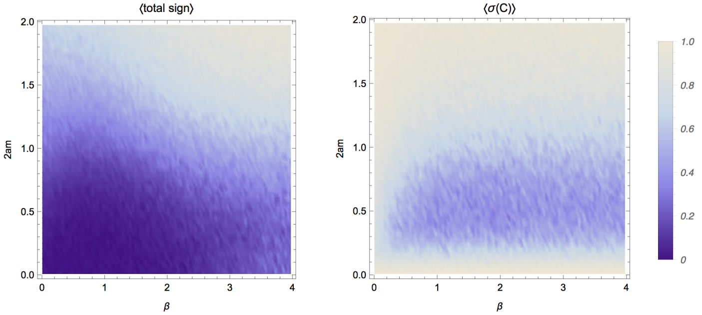
The **sign** s has a **fermionic** σ_F and a **bosonic** σ_B contribution:

$$s = \underbrace{(-1)^{N_-(C)+w_\tau(C)+1} \prod_{(x,\mu)\in C} \eta_{x\mu}}_{\sigma_F(C)} \times \underbrace{\mathrm{sign}\left(\prod_{i=1}^{\#C} 2\mathrm{Re}(\mathcal{U}(C_i))\right)}_{\sigma_B(C)}$$



which behave very differently...

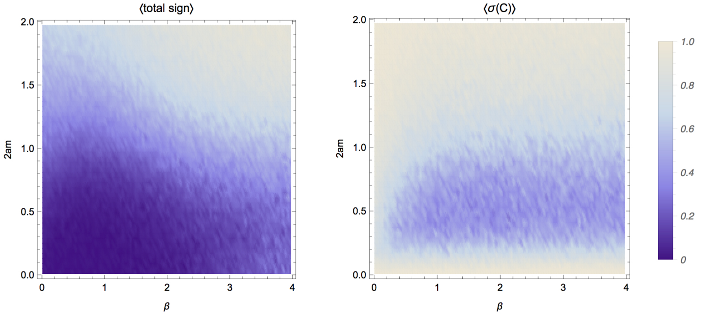
8×8 **lattice**



- **Problem:** Electron loop holonomies fluctuate very close to zero near $\beta \approx 0$, which artificially enhances the bosonic sign.
- **Solution:** (?) Integrate bosonic d.o.f. numerically *a priori*, use exact loop expansion of $\det \not{D}$ to weight electron loops $\Rightarrow$ only σ_F would survive:

$$Z(\beta, m) = Z_g(\beta) \sum_{\{n,k,C\}} \sigma_F(C) \prod_x (2am)^{n_x} \prod_{x,\mu} \xi_\mu^{2k_{x\mu}} \underbrace{\left\langle \prod_{i=1}^{\#C} 2\mathrm{Re}(U(C_i)) \right\rangle_g}_{>0}$$

8×8 **lattice**



Conclusions

- The representation of lattice gauge theories without link variables provides a diagrammatic representation of compact lattice QED (and non-Abelian gauge theories) amenable to Monte Carlo simulations with worm-like algorithms.
- We simulate a monomer-dimer-loop representation of compact lattice QED $N_f = 1$ as a toy model for the non-Abelian and/or multi-flavor case.
- We benchmarked our simulation algorithm with simple analytical results
- The sign problem has both a bosonic and a fermionic origin, in which the former becomes severe at $\beta \approx 0$.
- A possible solution to the bosonic sign problem may reside in either:
  - the numerical integration of the bosonic d.o.f. for any β
  - the analytic integration of the bosonic d.o.f. in a strong coupling expansion