Lattice QED with dual variables

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Introduction

- **Goal:** Ab initio simulations of **eXtreme QCD** (at finite density and temperature), with a **modest sign problem**: Taming the sign rather than killing it.

- **What is the sign problem?**
  - In lattice QCD, fermion fields are integrated out first $\Rightarrow$ $\det\left(\not{D}\right)$
  - At finite density μ, $\det\left(\not{D}(\mu)\right)$ is **complex-valued**, *i.e.* the probabilistic interpretation in Euclidean space is lost.
  - However, the sign problem is **basis-dependent**, *e.g.* it does not exist in the eigenbasis of any quantum Hamiltonian:

$$Z = \mathrm{Tr}\; e^{-\beta \hat{H}} = \mathrm{Tr}\Big\{ e^{-\frac{\beta}{N}\hat{H}} \sum\nolimits_i |\Psi_i\rangle\langle\Psi_i| e^{-\frac{\beta}{N}\hat{H}} \sum\nolimits_j |\Psi_j\rangle\langle\Psi_j| \cdots \Big\}$$

$$\langle\Psi_i|e^{-\beta\hat{H}}|\Psi_j\rangle \geq 0,\ \forall i,j$$

- **Technical goal:** To find a suitable basis for the partition sum of lattice QCD, in which the sign problem becomes sufficiently mild.
  - Sensible candidates are the **color-neutral** fermionic states obtained after integrating out the gauge fields $\approx$ asymptotic confined states of QCD.

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$SU(N_c)$ lattice QCD, at $\beta = 0$

In $SU(N_c)$ lattice QCD, analytical integration of $U_{x\mu}$ ***before*** $\psi_x, \bar{\psi}_x$ is possible at $\beta = 0$ $\Rightarrow$ **monomer-dimer-loop** system [Rossi-Wolff '84]

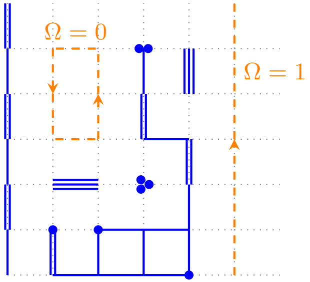
$$Z = \int \mathcal{D}U \mathcal{D}\psi \mathcal{D}\bar{\psi}\; e^{2am\sum_x \mathrm{Tr}(\bar{\psi}_x\psi_x) + \sum_{x,\mu}\eta_{x\mu}\mathrm{Tr}\left(e^{a\mu}\bar{\psi}_x U_{x\mu}\psi_{x+\hat{\mu}} - e^{-a\mu}\bar{\psi}_x U_{x\mu}\psi_{x+\hat{\mu}}\right)}$$

$$= \sum_{\{n,k,\ell\}} \frac{\sigma(\ell)}{N_c!^{|\ell|}} e^{N_c N_t a\mu\Omega(\ell)} \left(\prod_x \frac{N_c!}{n_x!}(2am)^{n_x}\right)\left(\prod_{x,\mu}\frac{(N_c - k_{x\mu})!}{N_c! k_{x\mu}!}\right)$$

- **Content:**
  $n_x, k_{x\mu} \in \{0, \ldots, N_c\}, \;\; \ell_{x\mu} \in \{0, \pm 1\}$
- **Grassmann constraints:**

  $$n_x + \sum_{\pm\mu}\left(k_{x\mu} + \frac{N_c}{2}|\ell_{x\mu}|\right) \overset{!}{=} N_c$$

- Configurations are generated using a **directed path (worm) algorithm**.
  [Adams-Chandrasekharan '03]



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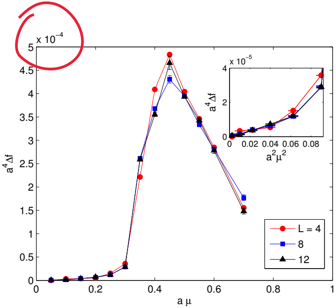
- **Baryonic sign problem:**
  $\sigma(\ell) = \pm 1$
- Quantitative measure of the severity of the sign problem:

  $$\langle \mathrm{sign} \rangle = Z/Z_{||} = e^{V\Delta f}$$
- For small μ, the sign problem is **milder** than in the traditional formulation of lattice QCD, by a factor $O(10^{-4})$.



$SU(N_c)$ lattice QCD, at $O(\beta)$

In $SU(N_c)$ lattice QCD, analytical integration of $U_{x\mu}$ ***before*** $\psi_x, \bar{\psi}_x$ is also possible order-by-order in β $\Rightarrow$ **monomer-dimer-loop-plaquette** system [Forcrand-Langelage-Philipsen-Unger '14]

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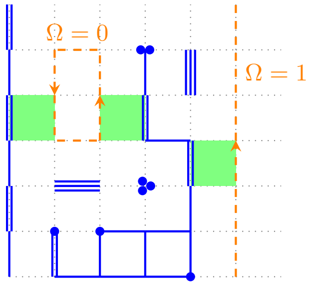
$$\times\left(1+\frac{\beta}{N_c}\sum_{\Box}\mathrm{ReTr}\left(U_\Box\right)\right)$$
$$= \sum_{\{n,k,\ell,p\}}\frac{\sigma(\ell)}{N_c!^{|\ell|}}e^{N_c N_t a\mu\Omega(\ell)}\left(\prod_x \frac{N_c! v_x}{n_x!}(2am)^{n_x}\right)\left(\prod_{x,\mu}\frac{(N_c-k_{x\mu})!}{N_c!(k_{x\mu}-p_{x\mu})!}\right)\prod_{\Box}\left(\frac{\beta}{2N_c}\right)^{p_\Box}$$

- **New content:**
  Plaquette occupation numbers, $p_{x\mu\nu}$
- **Grassmann constraints:**

  $$n_x + \sum_{\pm\mu} k_{x\mu} \overset{!}{=} N_c + \sum_{\mu<\nu} p_{x\mu\nu}$$
- Configurations are generated using a **directed path (worm) algorithm**.
  [Adams-Chandrasekharan '03]



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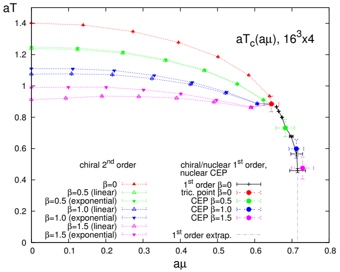
$$= \sum_{\{n,k,\ell,p\}} \frac{\sigma(\ell)}{N_c!^{|\ell|}} e^{N_c N_t a\mu \Omega(\ell)} \left(\prod_x \frac{N_c! v_x}{n_x!} (2am)^{n_x}\right) \left(\prod_{x,\mu} \frac{(N_c - k_{x\mu})!}{N_c!(k_{x\mu} - p_{x\mu})!}\right) \prod_\Box \left(\frac{\beta}{2N_c}\right)^{p_\Box}$$

- The sign problem is mild enough to allow the mapping of the full phase diagram of strongly-coupled lattice QCD. [Forcrand-Langelage-Philipsen-Unger '14]

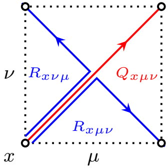
- But, beyond $O(\beta)$, it becomes combinatorially hard to control the necessary diagrammatics. [Unger '16]
A new approach is required!



Integrating out the link variables

Use **auxiliary bosonic fields** to decouple the links around plaquettes: [Forcrand-HV '14]

$$Z = \int \prod_{x,\mu} dU_{x\mu}\, e^{\frac{\beta}{N_c}\sum_{\Box} \mathrm{ReTr}(UUUU)}$$

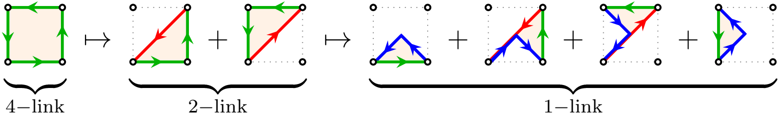


1. Add two sets of auxiliary bosonic fields living on plaquettes, $Q_{x\mu\nu}$ and $R_{x\mu\nu}$ (Gaussian).

2. Use **Hubbard-Stratonovich transformations** to decouple all links:

$$Q_{x\mu\nu} \mapsto \sqrt{\frac{\beta}{N_c}}(Q_{x\mu\nu} + U_{x\mu}U_{x+\hat{\mu},\nu} + U_{x\nu}U_{x+\hat{\nu},\mu})$$

$$R_{x\mu\nu} \mapsto \sqrt{\frac{\beta}{N_c}}(R_{x\mu\nu} + Q_{x\mu\nu}U^{\dagger}_{x+\hat{\mu},\nu} + U_{x\mu})$$



Integrating out the link variables

The Wilson plaquette action **becomes linear**, and so the partition sum factorizes as a product of exactly solvable **one-link integrals**:

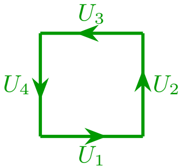
$$Z = \int \mathcal{D}Q\,\mathcal{D}R\, e^{-\frac{3\beta}{2N_c}\mathrm{Tr}(QQ^\dagger)-\frac{\beta}{2N_c}\mathrm{Tr}(RR^\dagger)} \left(\prod_{x,\mu}\int dU\, e^{\frac{\beta}{N_c}\mathrm{Re}\mathrm{Tr}(J^\dagger_{x\mu}U)}\right)$$

$J_{x\mu}$ only depends on the auxiliary fields,

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

Wilson loops are path-ordered products of **effective links**, $\widetilde{U}_l$:

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



$$\widetilde{U}_l = \int dU\, U\, e^{\beta\mathrm{Re}(J_l^\dagger U)}$$

Compact $U(1)$ lattice gauge theory

In pure $U(1)$ lattice gauge theory, the 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**:

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

The representation of the partition sum without link variables (**0-link**) is:

$$Z = \int \mathcal{D}U \prod_{\Box} e^{\beta \mathrm{Re}(U_\Box)} = \int \mathcal{D}Q\, \mathcal{D}R\, e^{-\frac{3\beta}{2}|Q|^2 - \frac{\beta}{2}|R|^2} \prod_l I_0(\beta |J_l|)$$

$U(1)$ **loop observables** in the 0-link representation,

$$\langle W(\ell) \rangle = \left\langle \prod_{l \in \ell} U_l \right\rangle = \left\langle \prod_{l \in \ell} \widetilde{U}_l \right\rangle$$

are defined in terms of $U(1)$ **effective links**:

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

Compact lattice QED

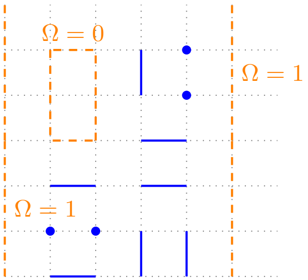
The generalization of this formalism to compact lattice QED is straightforward:

$$Z = \int \mathcal{D}\psi\, \mathcal{D}\bar{\psi} e^{2am\bar{\psi}\psi} \int \mathcal{D}Q\, \mathcal{D}R\, e^{-\frac{3\beta}{2}|Q|^2 - \frac{\beta}{2}|R|^2} \prod_{x,\mu} \int dU\, e^{\mathrm{Re}\left(\left(\beta J^{\dagger}_{x\mu} + 2\eta_{x\mu}\psi_x \psi_{x+\hat{\mu}}\right)^{\dagger} U\right)}$$

$$= \int \mathcal{D}Q\, \mathcal{D}R\, e^{-\frac{3\beta}{2}|Q|^2 - \frac{\beta}{2}|R|^2} \prod_{l} I_0(\beta|J_l|) \sum_{\{n,k,\ell\}} (2am)^{N_M} \sigma_F(\ell) \prod_{i=1}^{\#\ell} 2\mathrm{Re}(W(\ell_i))$$

- **Sign problem(s):** $\sigma_F(\ell) = \pm 1$, but $\mathrm{Re}(W(\ell_i))$ can also be negative!
- **Grassmann constraints:**

  $n_x + \sum_{\pm\mu} \left(k_{x\mu} + \frac{N_c}{2}|\ell_{x\mu}|\right) \stackrel{!}{=} 1$
- **Gauss' law:** Only the zero-winding sector contributes



Monte Carlo algorithm

1. **Gaussian heatbath**, for (Q, R)
   + **HS transformations**, with the help of an auxiliary $U(1)$ field
   + **Metropolis**, for the electron loop corrections:

$$\underbrace{\mathcal{D}Q\,\mathcal{D}R\,e^{-\frac{3\beta}{2}\mathrm{Tr}(QQ^\dagger)-\frac{\beta}{2}\mathrm{Tr}(RR^\dagger)}\prod_l I_0(\beta|J_l|)}_{\text{Heatbath (local)}}\underbrace{\prod_{i=1}^{\#\ell} 2\,\mathrm{Re}(W(\ell_i))}_{\text{Metropolis (global)}}$$

2. **"Mesonic" worm**, for the monomer-dimer cover:
   [Prokof'ev-Svistunov '01] [Adams-Chandrasekharan '03]

$$w = \prod_x (2am)^{n_x} \prod_l 1$$

3. **Electron worm**, for (unoriented) electron loops, and dimers:

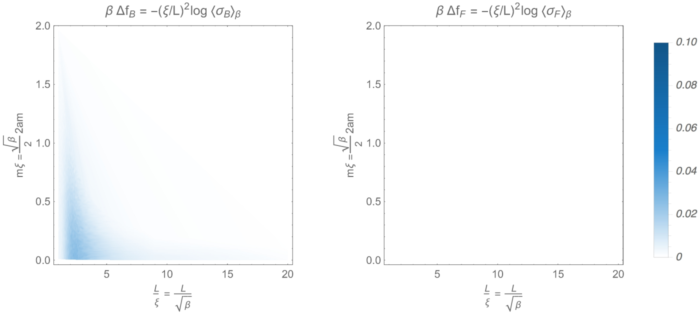
$$w = \prod_l 1 \prod_{i=1}^{\#\ell} |2\mathrm{Re}(W(\ell_i))| = \underbrace{\prod_l \left(\frac{I_1(\beta|J_l|)}{I_0(\beta|J_l|)}\right)^{\ell_l}}_{\text{Worm (local)}}\underbrace{\prod_{i=1}^{\#\ell} |2\cos(\arg(W(\ell_i)))|}_{\text{Metropolis (global)}}$$

Sign problem(s)

The **sign** $\sigma(\ell)$ has a **bosonic** $\sigma_B(\ell)$ and a **fermionic** $\sigma_F(\ell)$ contribution:

$$\sigma(\ell) = \sigma_B(\ell)\,\sigma_F(\ell) = \text{sign}\left(\prod_{i=1}^{\#\ell} 2\,\text{Re}(W(\ell_i))\right)(-1)^{N_-(\ell)+\omega_t(\ell)+1}\prod_{l\in\ell}\eta_l$$

2×2 lattice



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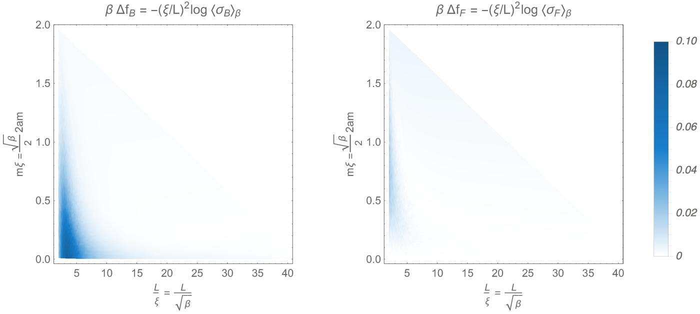
4×4 lattice



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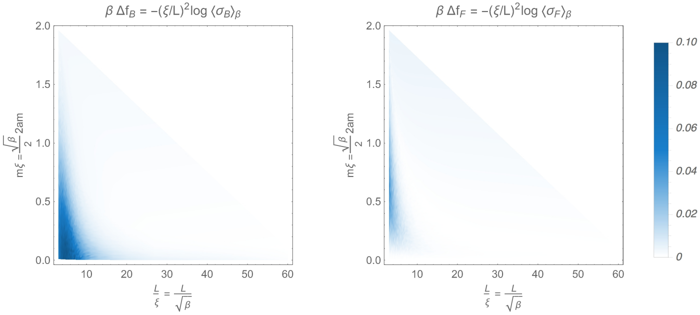
6 × 6 lattice



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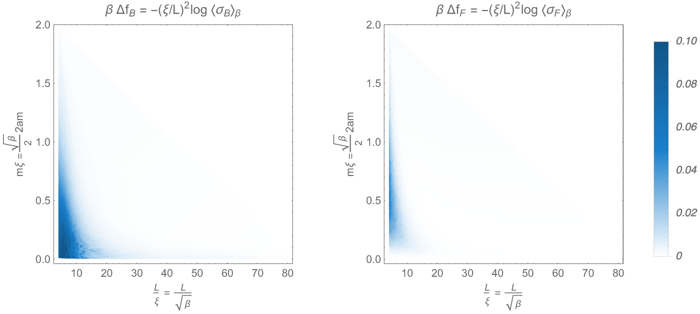
8 × 8 lattice



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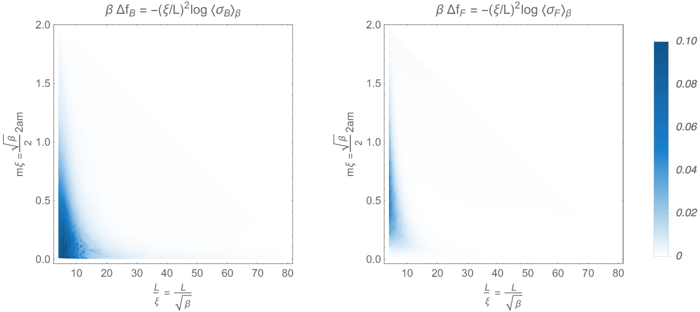

Origin: Negative tail of the distribution of $W(\ell_i)$ at $\beta \approx 0$

Solution: Integrating out oscillating d.o.f. $\Rightarrow$ variance reduction

Solution of the bosonic sign problem for $U(1)$

- Consider the linearized form of the partition sum (pure gauge theory):

$$Z = \int \mathcal{D}Q\,\mathcal{D}R\,\mathcal{D}U\, e^{-\frac{3\beta}{2}|Q|^2 - \frac{\beta}{2}|R|^2 + \beta\sum_{x,\mu}\mathrm{Re}(J_{x\mu}U^\dagger_{x\mu})}$$

- In order to reduce the variance from fluctuations of Q, R, U, **integrate the complex phases** analytically:

$$Q_{x\mu\nu} = |Q_{x\mu\nu}|\, e^{i\psi_{x\mu\nu}}, \qquad R_{x\mu\nu} = |R_{x\mu\nu}|\, e^{i\varphi_{x\mu\nu}}, \qquad U_{x\mu} = e^{i\theta_{x\mu}}$$

$$J_{x\mu} = \sum_{\nu\neq\mu}\left(|R_{x-\hat{\nu},\nu\mu}||Q_{x-\hat{\nu},\nu\mu}|e^{i(\psi_{x-\hat{\nu},\nu\mu}-\varphi_{x-\hat{\nu},\nu\mu})} + |R_{x\mu\nu}|e^{i\varphi_{x\mu\nu}}\right)$$

- First, let the R-phases absorb the U-phases: $\varphi_{x\mu\nu} \leftarrow \varphi_{x\mu\nu} - \theta_{x\mu}$
  The Boltzmann weight thus becomes:

$$\begin{aligned} e^{-S} &= e^{\beta\sum_{x,\mu}\mathrm{Re}(J_{x\mu}U^\dagger_{x\mu})} \\ &= \prod_{x,\mu\neq\nu} e^{\beta\left(|R_{x\nu\mu}||Q_{x\nu\mu}|\cos(\psi_{x\nu\mu}-\varphi_{x\nu\mu}-\theta_{x+\hat{\nu},\mu}-\theta_{x\nu})+|R_{x\mu\nu}|\cos(\varphi_{x\mu\nu})\right)} \end{aligned}$$

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$$\begin{aligned} e^{-S} &= e^{\beta \sum_{x,\mu} \mathrm{Re}(J_{x\mu} U^\dagger_{x\mu})} \\ &= \prod_{x,\mu\neq\nu} e^{\beta\left(|R_{x\nu\mu}||Q_{x\nu\mu}| \cos(\psi_{x\nu\mu} - \varphi_{x\nu\mu} - \theta_{x+\hat{\nu},\mu} - \theta_{x\nu}) + |R_{x\mu\nu}| \cos(\varphi_{x\mu\nu})\right)} \end{aligned}$$

Solution of the bosonic sign problem for $U(1)$

- Using: $e^{z\cos\alpha} = \sum_p I_p(z)\, e^{ip\alpha}$, and integrating out the Q-phases:

$$\int [d\psi]\, e^{-S} = \prod_{x,\mu<\nu} \Big\{ e^{\beta|R_{x\mu\nu}|\cos(\varphi_{x\mu\nu})} e^{\beta|R_{x\nu\mu}|\cos(\varphi_{x\nu\mu})} \times \sum_{p_{x\mu\nu}} I_{p_{x\mu\nu}}\left(\beta|R_{x\mu\nu}||Q_{x\mu\nu}|\right) I_{p_{x\mu\nu}}\left(\beta|R_{x\nu\mu}||Q_{x\mu\nu}|\right) \times e^{ip_{x\mu\nu}(\varphi_{x\nu\mu}-\varphi_{x\mu\nu}-\theta_{x\mu\nu})} \Big\}$$

where $\theta_{x\mu\nu} = \theta_{x\mu} + \theta_{x+\hat{\mu},\nu} - \theta_{x+\hat{\nu},\mu} - \theta_{x\nu}$ is the phase of a plaquette.

- The integration of the U-phases yields:

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and imposes a constraint on the p's:

$$\sum_{\nu\neq\mu}(p_{x-\hat{\nu},\nu\mu} - p_{x\nu\mu}) \stackrel{!}{=} 0$$

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Solution of the bosonic sign problem for $U(1)$

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- The full partition sum of lattice QED then becomes:

$$Z = \sum_{\{n,k,\ell,p\}} \sigma_F(\ell)\,(2am)^{N_M} \int_{[0,\infty)} \mathcal{D}|Q|^2\, \mathcal{D}|R|^2\, e^{-\frac{3\beta}{2}|Q|^2 - \frac{\beta}{2}|R|^2}$$
$$\times \prod_{x,\mu\neq\nu} I_{p_{x\mu\nu}}\left(\beta |R_{x\nu\mu}||Q_{x\mu\nu}|\right) I_{p_{x\mu\nu}}\left(\beta |R_{x\mu\nu}|\right)$$

  which has **no bosonic sign problem!**

- In the presence of fermion loops, the sum of p's around a link is compensated by the fermionic content on that link:

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Solution of the bosonic sign problem for $U(1)$

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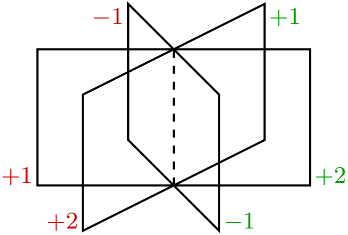
Solution of the bosonic sign problem for $U(1)$

Admissible plaquette configurations in the pure $U(1)$ gauge theory:

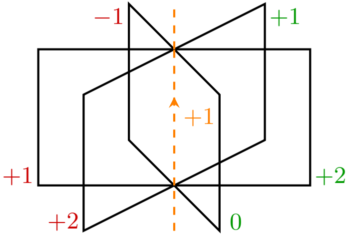
$$\sum_{\nu \neq \mu} (p_{x-\hat{\nu},\nu\mu} - p_{x\nu\mu}) \stackrel{!}{=} 0$$



Solution of the bosonic sign problem for $U(1)$

Admissible plaquette configurations in compact lattice QED:

$$\sum_{\nu \neq \mu} (p_{x-\hat{\nu},\nu\mu} - p_{x\nu\mu}) \stackrel{!}{=} \ell_{x\mu}$$



Proposed Monte Carlo algorithm

(in progress)

1. **Bosonic updates:**
   - **"Exponential" heatbath** + **Metropolis**, for $(|Q_{x\mu\nu}|^2, |R_{x\mu\nu}|^2)$:

$$P_{Q_{x\mu\nu}\to Q'_{x\mu\nu}} = \frac{I_{p_{x\mu\nu}}(\beta|Q'_{x\mu\nu}||R_{x\mu\nu}|)\, I_{p_{x\mu\nu}}(\beta|Q'_{x\mu\nu}||R_{x\nu\mu}|)}{I_{p_{x\mu\nu}}(\beta|Q_{x\mu\nu}||R_{x\mu\nu}|)\, I_{p_{x\mu\nu}}(\beta|Q_{x\mu\nu}||R_{x\nu\mu}|)}$$

$$P_{R_{x\mu\nu}\to R'_{x\mu\nu}} = \frac{I_{p_{x\mu\nu}}(\beta|Q_{x\mu\nu}||R'_{x\mu\nu}|)\, I_{p_{x\mu\nu}}(\beta|R'_{x\mu\nu}|)}{I_{p_{x\mu\nu}}(\beta|Q_{x\mu\nu}||R_{x\mu\nu}|)\, I_{p_{x\mu\nu}}(\beta|R_{x\mu\nu}|)}$$

   - **"Mesonic" worm**, for the monomer-dimer cover:

$$w(n,k) = \prod_x (2am)^{n_x} \prod_l 1$$

2. **Fermionic updates:**
   - In $d = 2$: **Electron worm**, for (oriented) electron loops
     \+ **Metropolis** for $p \equiv p_{x\mu\nu}$:

$$P_{p\to p'} = \frac{I_{p'}(\beta|Q_{x\mu\nu}||R_{x\mu\nu}|)\, I_{p'}(\beta|Q_{x\mu\nu}||R_{x\nu\mu}|)\, I_{p'}(\beta|R_{x\mu\nu}|) I_{p'}(\beta|R_{x\nu\mu}|)}{I_{p}(\beta|Q_{x\mu\nu}||R_{x\mu\nu}|)\, I_{p}(\beta|Q_{x\mu\nu}||R_{x\nu\mu}|)\, I_{p}(\beta|R_{x\mu\nu}|) I_{p}(\beta|R_{x\nu\mu}|)}$$

   - In $d > 2$: **Surface worm**, for $p_{x\mu\nu}$ and (oriented) electron loops.

Summary and outlook

- The analytical integration of color d.o.f. in $SU(N_c)$ lattice QCD with staggered quarks can be done order-by-order in a strong coupling expansion: it reduces the severity of the sign problem by $O(10^{-4})$, but the integration becomes increasingly difficult beyond $O(\beta)$.
- The analytical integration of the lattice gauge and fermionic fields in compact lattice QED can be done for any value of β, at the cost of introducing auxiliary bosonic fields.
- Fluctuations of the auxiliary bosonic d.o.f. at $\beta \approx 0$ induce a bosonic sign problem, in addition to the sign problem due to the shape and topology of fermionic loops.
- The analytical integration of the phases of the auxiliary fields solves the bosonic sign problem in lattice QED.

Next:

- Severity of the remaining fermionic sign problem?
- Dual representation, and variance reduction, for $SU(2)$, $SU(3)$