Progress toward QCD at non-zero matter density

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Monte Carlo: no pain, no gain...

Monte Carlo highly efficient: *importance sampling* $\mathrm{Prob(conf)} \propto \exp(-E(\mathrm{conf})/T)$

- But all low-hanging fruits have been picked by now
- Further progress requires tackling the sign problem
- Examples:

- real-time quantum evolution:

  weight in path integral $\propto \exp(-\frac{i}{\hbar} Ht) \longrightarrow$ phase cancellations

- Hubbard model:

  repulsion $U n_\uparrow n_\downarrow \underset{\text{Hubbard-Stratonovich}}{\rightarrow} \det_\uparrow \det_\downarrow$

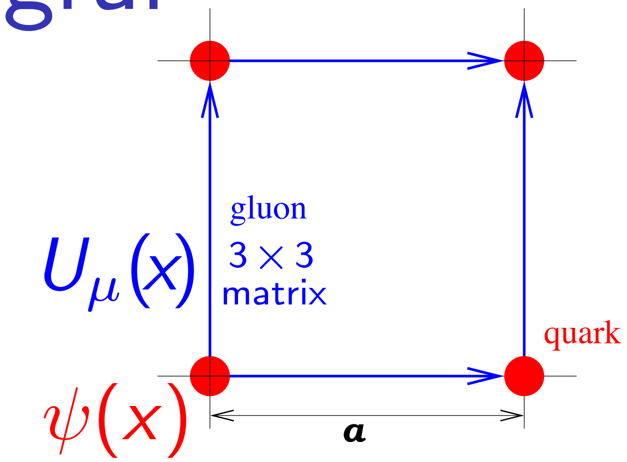
  complex except at half-filling (additional symmetry)

- QCD at non-zero density / chemical potential:

  integrate out the fermions $\det(\not{D} + \mu\gamma_0)^2$ $(N_f = 2)$

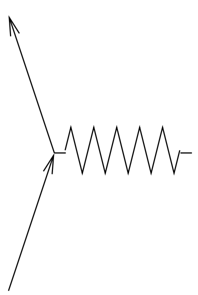
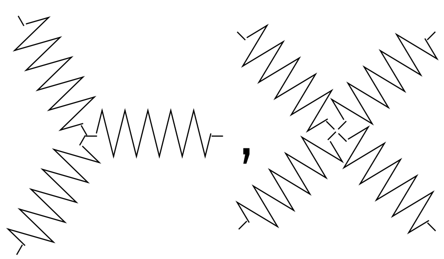
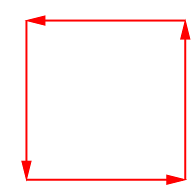
  complex unless $\mu = 0$ or pure imaginary (additional symmetry)

Lattice QCD: Euclidean path integral



space + imag. time $\rightarrow$ $4d$ hypercubic grid:

$$Z = \int \mathcal{D}U\mathcal{D}\bar{\psi}\mathcal{D}\psi e^{-S_E[\{U,\bar{\psi},\psi\}]}$$

- Discretized action S_E:
  -  $\longrightarrow$ $\bar{\psi}(x)U_\mu(x)\psi(x+\hat{\mu}) + h.c.,$ Dirac operator $\bar{\psi}\not{D}\,\psi$
  -  $\longrightarrow$ $\beta\,\mathrm{ReTr}U_P$, U_P plaquette matrix  Yang-Mills action $\frac{1}{4}F_{\mu\nu}F_{\mu\nu}$

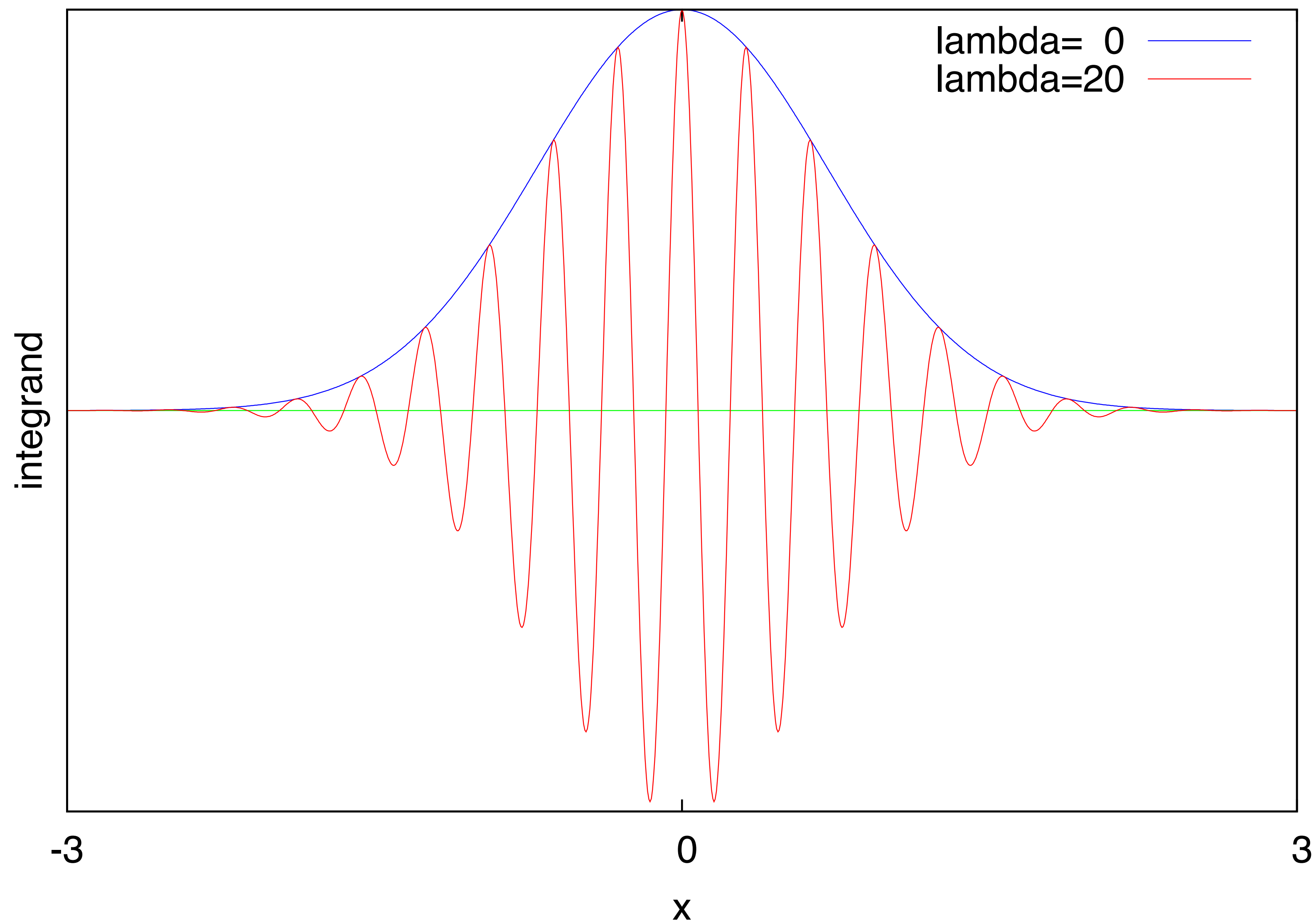
$$a \rightarrow 0 \Leftrightarrow \beta = \frac{6}{g_0^2} \rightarrow \infty$$

- Monte Carlo: with Grassmann variables $\psi(x)\psi(y) = -\psi(y)\psi(x)$??
  Integrate out analytically (Gaussian) $\rightarrow$ determinant *non-local*

$$\mathrm{Prob}(\mathrm{config}\{U\}) \propto \det{}^2 \not{D}(\{U\})\; e^{+\beta\sum_P \mathrm{ReTr}U_P}$$ real non-negative when $\mu = 0$

Sampling oscillatory integrands

- Example: $Z(\lambda) = \int dx \exp(-x^2 + \mathbf{i\lambda x}) = \int dx \exp(-x^2)\cos(\lambda x)$



- $Z(\lambda)/Z(0) = \exp(-\lambda^2/4)$: exponential cancellations

$\rightarrow$ truncating deep in the tail at $x \sim \lambda$ gives $\mathcal{O}(100\%)$ error

"Every x is important" $\leftrightarrow$ How to sample?

Computational complexity of the sign pb

- How to study: $Z_\rho \equiv \int dx\ \rho(x), \quad \rho(x) \in \mathbf{R}$, with $\rho(x)$ sometimes negative ?

  Reweighting: sample with $|\rho(x)|$, and "put the sign in the observable":

$$\langle W \rangle_f \equiv \frac{\int dx\ W(x)\rho(x)}{\int dx\ \rho(x)} = \frac{\int dx\ [W(x)\mathrm{sign}(\rho(x))]\ |\rho(x)|}{\int dx\ \mathrm{sign}(\rho(x))\ |\rho(x)|} = \boxed{\frac{\langle W\mathrm{sign}(\rho)\rangle_{|\rho|}}{\langle \mathrm{sign}(\rho)\rangle_{|\rho|}}}$$

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- $\langle \mathrm{sign}(\rho)\rangle_{|\rho|} = \frac{\int dx\ \mathrm{sign}(\rho(x))|\rho(x)|}{\int dx\ |\rho(x)|} = \boxed{\frac{Z_\rho}{Z_{|\rho|}}} = \exp(-\frac{V}{T}\underbrace{\Delta f(\mu^2, T)}_{\text{diff. free energy dens.}})$, exponentially small

  Each meas. of $\mathrm{sign}(\rho)$ gives value $\pm 1 \Longrightarrow$ statistical error $\approx \frac{1}{\sqrt{\#\ \text{meas.}}}$

  Constant relative accuracy $\Longrightarrow$ **need statistics $\propto \exp(+2\frac{V}{T}\Delta f)$**

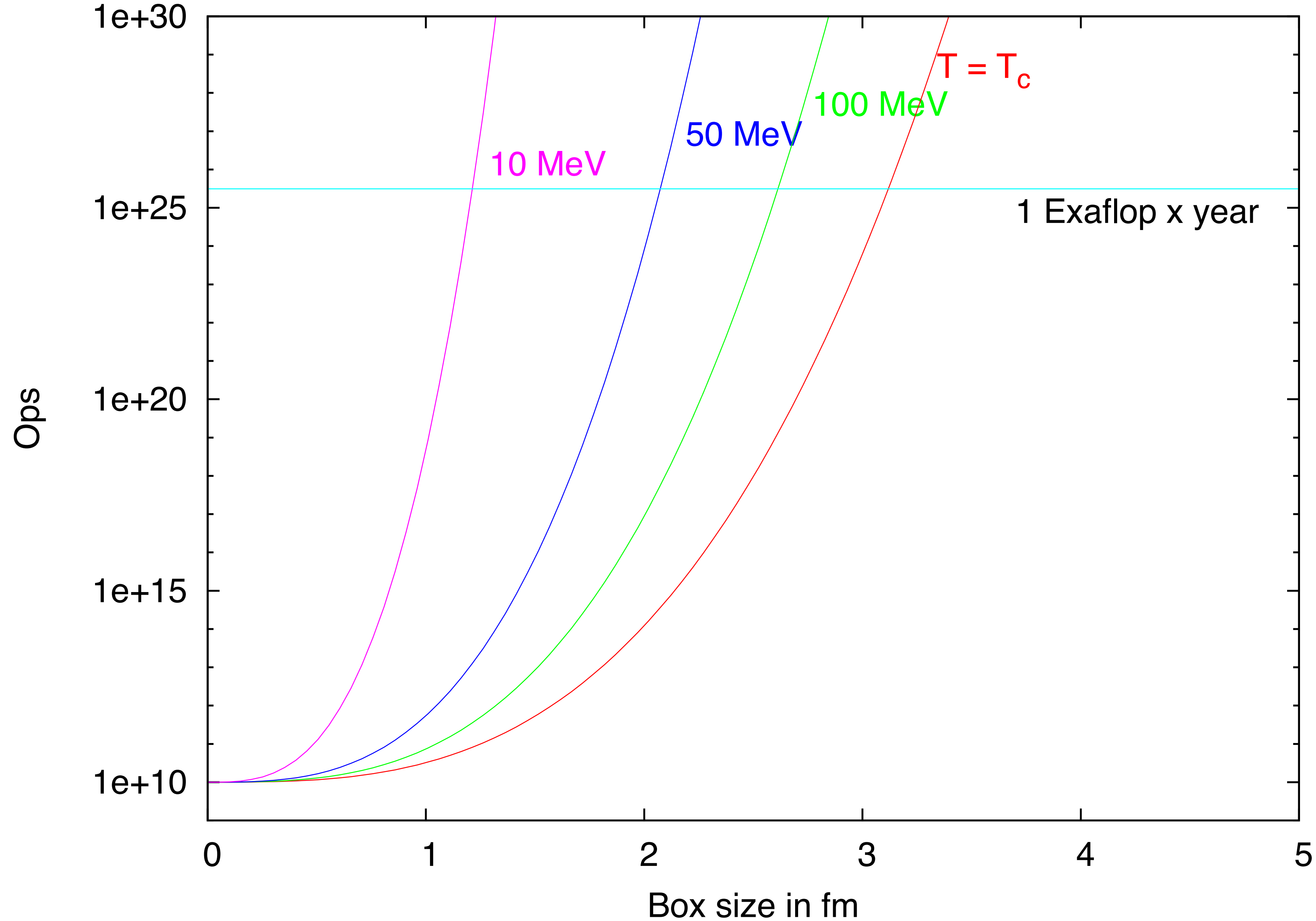
  Large V, low T inaccessible: signal/noise ratio degrades exponentially

Δf measures severity of sign pb.

"Sign problem" is generic roadblock: condensed matter, real time, $\cdots$

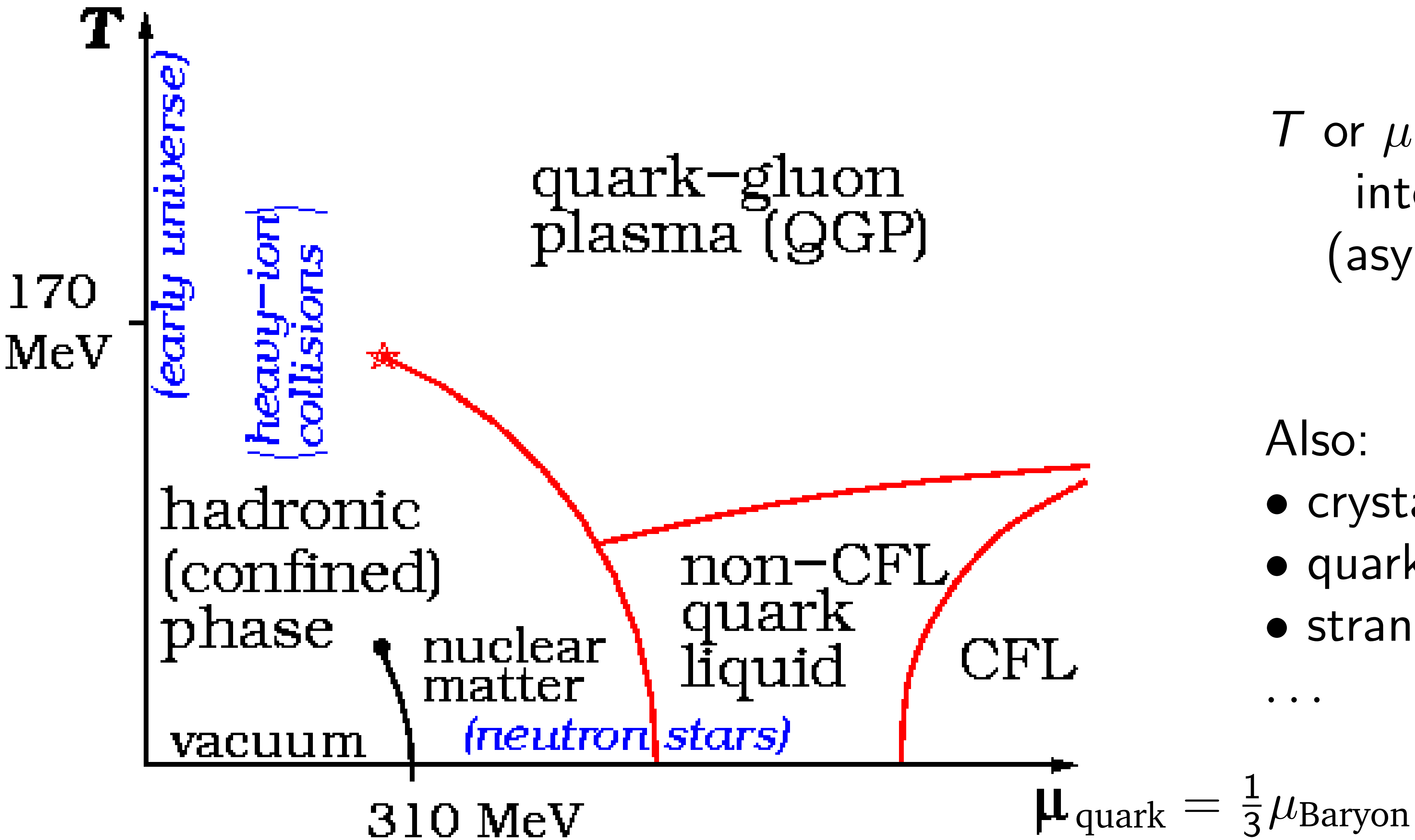
The CPU effort grows *exponentially* with L^3/T

CPU effort to study matter at nuclear density in a box of given size
Give or take a few powers of 10...



Crudely based on:
- 1 sec on 1GF laptop for 2^4 lattice, $a = 0.1$ fm
- effort $\propto \exp(2\frac{V}{T}\underbrace{\rho_{\text{nucl.}}(m_B - 3/2m_\pi)}_{\Delta f})$

Reward prospects: the wonderland phase diagram of QCD from Wikipedia



T or $\mu \to \infty$:
interaction weak
(asymptotic freedom)

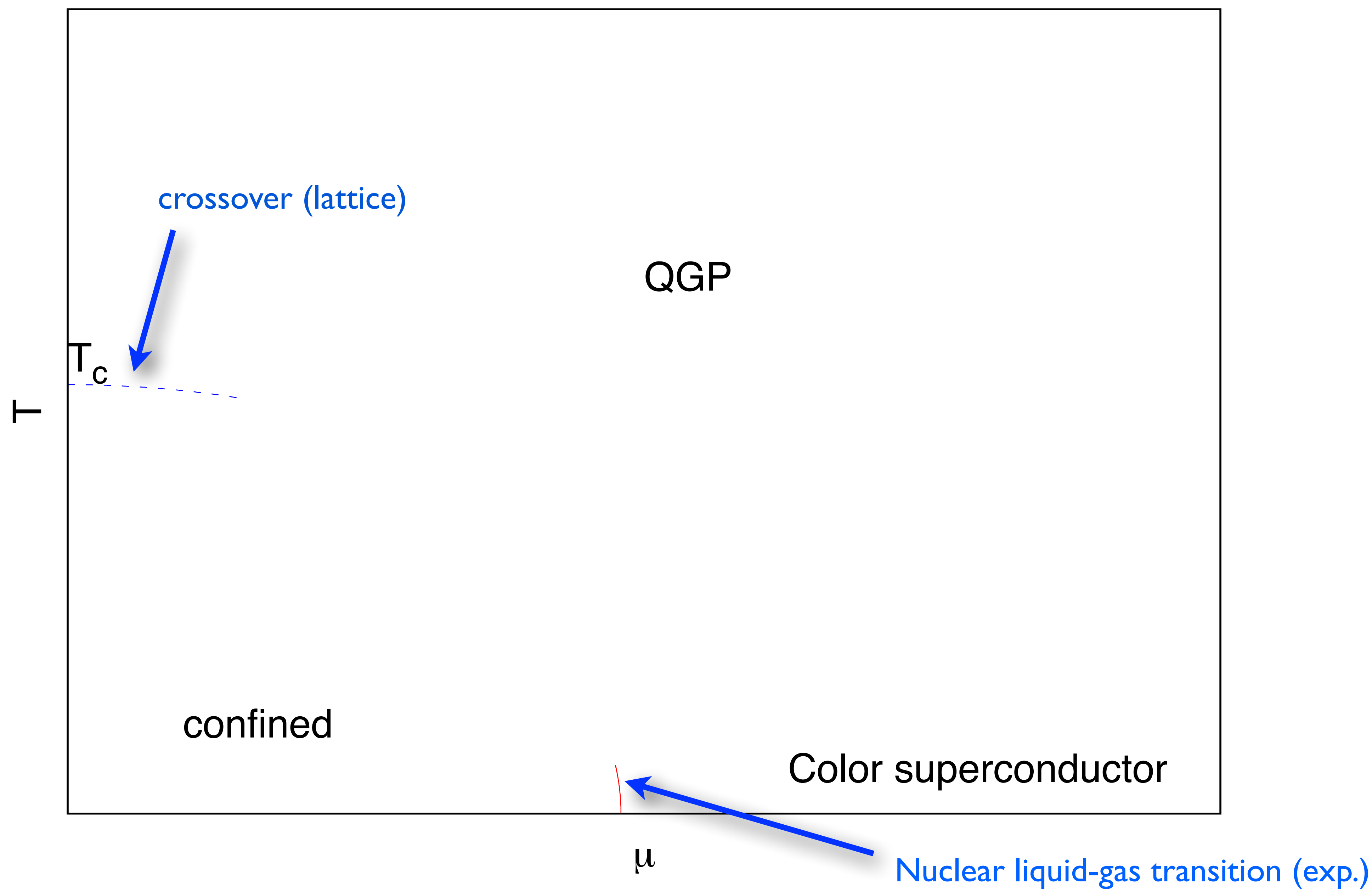
Also:

- crystal phase(s)
- quarkyonic phase
- strangelets

...

Caveat: everything in red is a conjecture

Finite μ: what is known?



Minimal, possible phase diagram

Frogs and birds

- Frogs: *acknowledge* the sign problem
  - explore region of small $\frac{\mu}{T}$ where sign pb is mild enough
  - find tricks to enlarge this region

- Birds: *solve* the sign pb
  - solve QCD ?
  - find a model which can be made sign-pb free and paint it “QCD-like”

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- *Think different*: build an analog QCD simulator with cold atoms

$\mu/T \gtrsim \mathcal{O}(1)$: how to make the sign problem milder?

- Severity of sign pb. is *representation dependent*:

$$Z = \mathrm{Tr} e^{-\beta H} = \mathrm{Tr}\left[e^{-\frac{\beta}{N}H}\left(\sum|\psi\rangle\langle\psi|\right)e^{-\frac{\beta}{N}H}\left(\sum|\psi\rangle\langle\psi|\right)\cdots\right]$$

Any complete set $\{|\psi\rangle\}$ will do

If $\{|\psi\rangle\}$ form an eigenbasis of H, then $\langle\psi_k|e^{-\frac{\beta}{N}H}|\psi_l\rangle = e^{-\frac{\beta}{N}E_k}\delta_{kl} \geq 0 \rightarrow$ no sign pb

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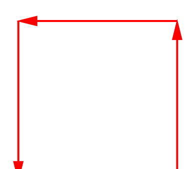
Usual:
- integrate over quarks analytically $\rightarrow \det(\{U\})$
- Monte Carlo over gluon fields $\{U\}$

Reverse order:
- integrate over gluons $\{U\}$ analytically
- Monte Carlo over quark color singlets (hadrons)

- Caveat: must turn off 4-link coupling  in $\beta\sum_P \mathrm{Re}\mathrm{Tr}\, U_P$ by setting $\beta = 0$

$\beta = \frac{6}{g_0^2} = 0$: strong-coupling limit $\longleftrightarrow$ continuum limit ($\beta \rightarrow \infty$)

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$$Z(\beta = 0) = \int \prod_x d\bar{\psi} d\psi \quad \prod_{x,\nu}\left(\int dU_{x,\nu} e^{-\{\bar{\psi}_x U_{x,\nu}\psi_{x+\hat{\nu}} - h.c.\}}\right)$$

Product of 1-link integrals performed analytically

Strong coupling limit at finite density (staggered quarks)

Chandrasekharan, Wenger, PdF, Unger, Wolff, ...

- Integrate over U's, then over quarks: *exact* rewriting of $Z(\beta = 0)$

New, discrete "*dual*" degrees of freedom: meson & baryon worldlines

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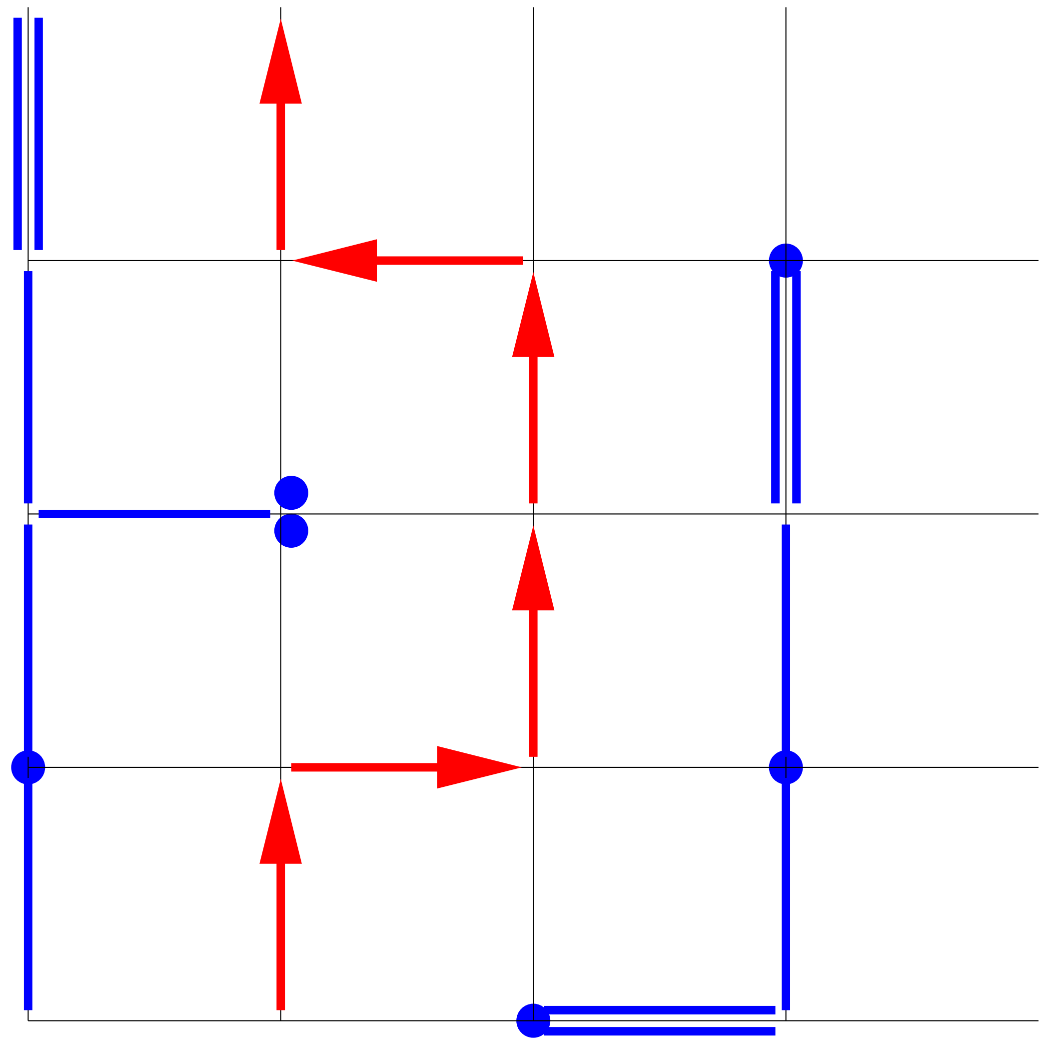

Constraint at every site:
3 blue symbols ($\bullet$ $\bar{\psi}\psi$, meson hop)
or a baryon loop

Update with worm algorithm: "*diagrammatic*" Monte Carlo

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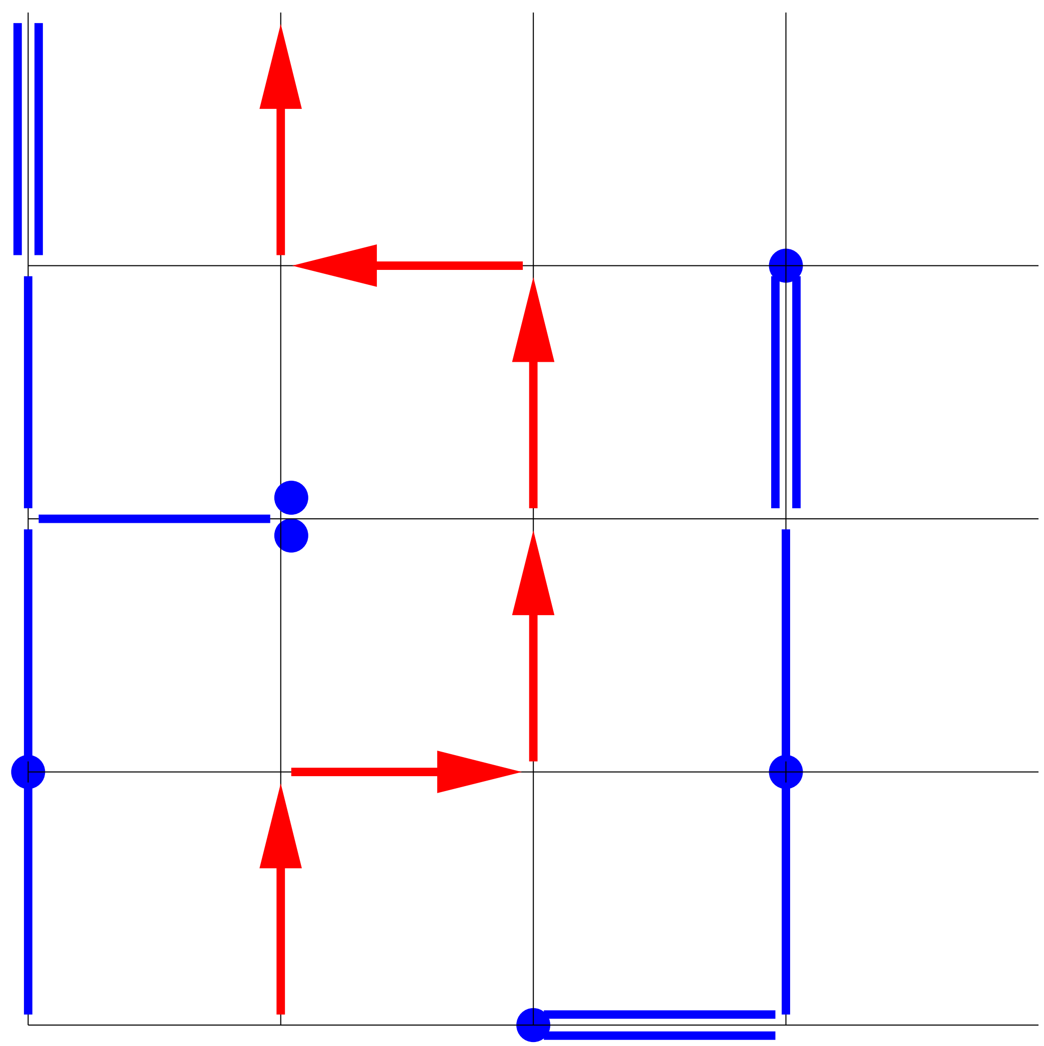

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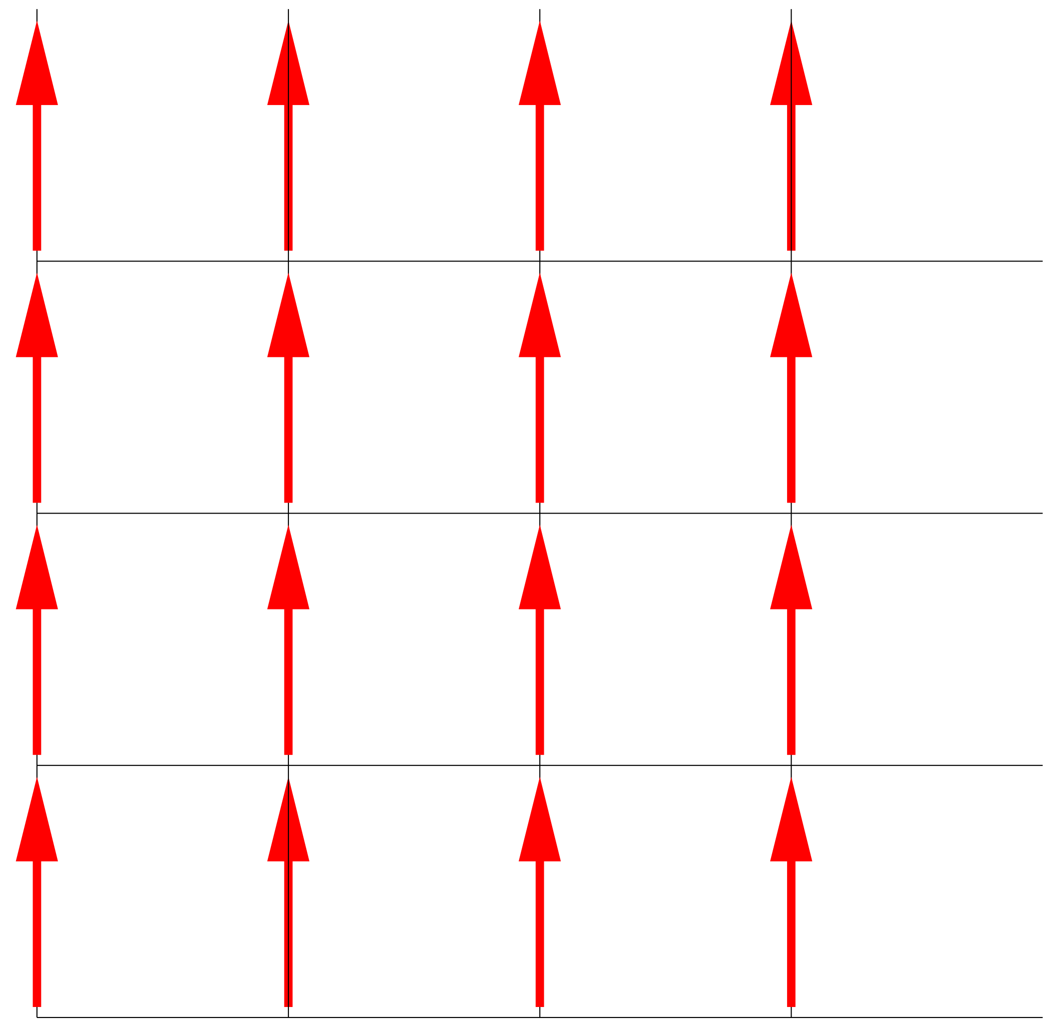
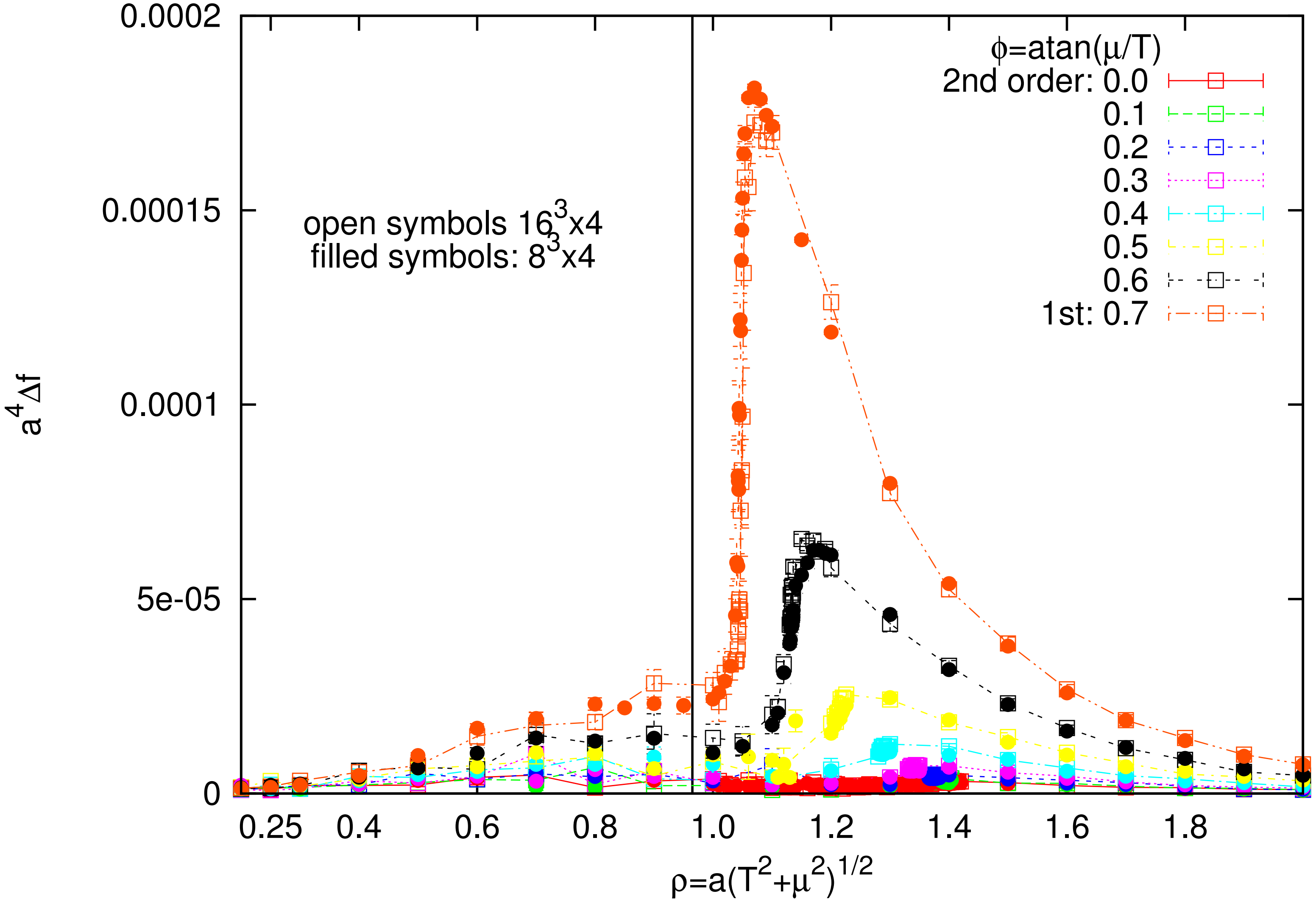


The dense (crystalline) phase:
1 baryon per site; no space left
$\rightarrow \quad \langle\bar\psi\psi\rangle = 0$

Update with worm algorithm: "*diagrammatic*" Monte Carlo

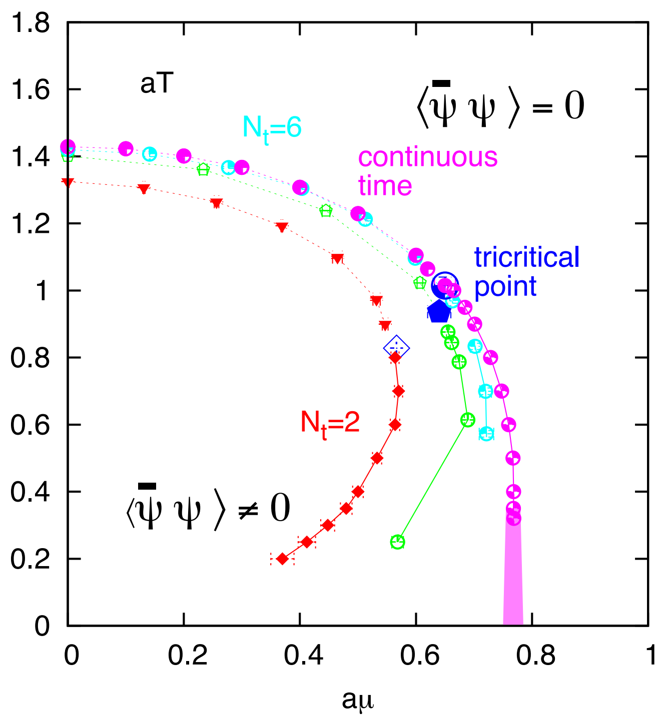
Sign problem? Monitor $\Delta f = -\frac{1}{V}\log\langle\mathrm{sign}\rangle$

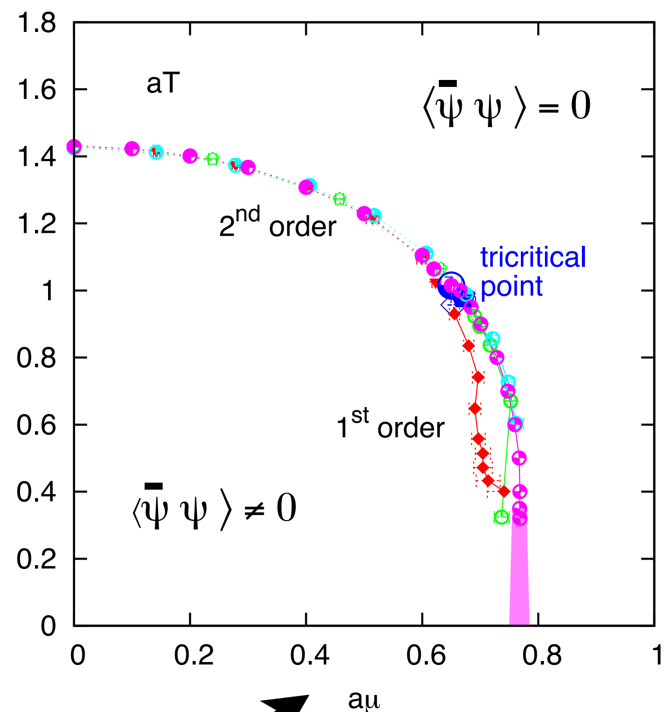


- $\langle\mathrm{sign}\rangle = \frac{Z}{Z_{||}} \sim \exp(-\frac{V}{T}\Delta f(\mu^2))$ as expected
- Determinant method $\rightarrow \Delta f \sim \mathcal{O}(1)$. Here, Gain $\mathcal{O}(10^4)$ in the exponent!
  - heuristic argument correct: color singlets closer to eigenbasis
  - negative sign? product of *local* neg. signs caused by spatial baryon hopping:
    - no baryon $\rightarrow$ no sign pb (no silver blaze pb.)
    - saturated with baryons $\rightarrow$ no sign pb

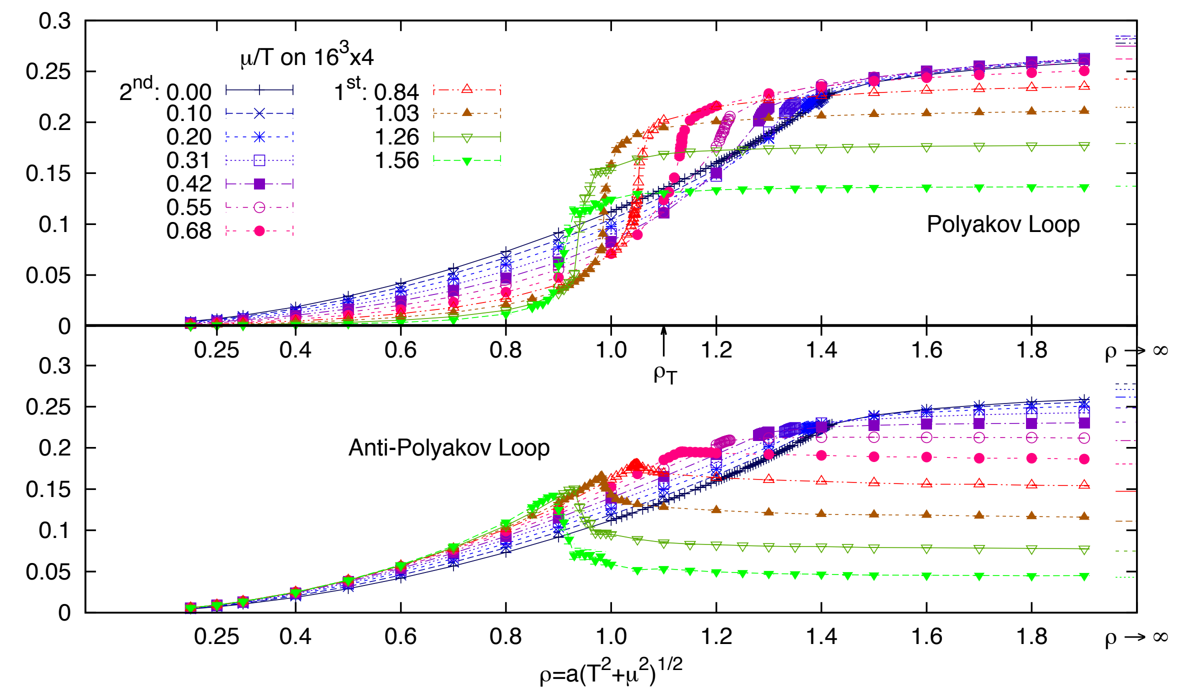
Results – Phase diagram and Polyakov loop ($m_q = 0$)

w/Unger, Langelage, Philipsen





$1/N_t^2$ corrections



Polyakov and anti-Polyakov loop vs mu

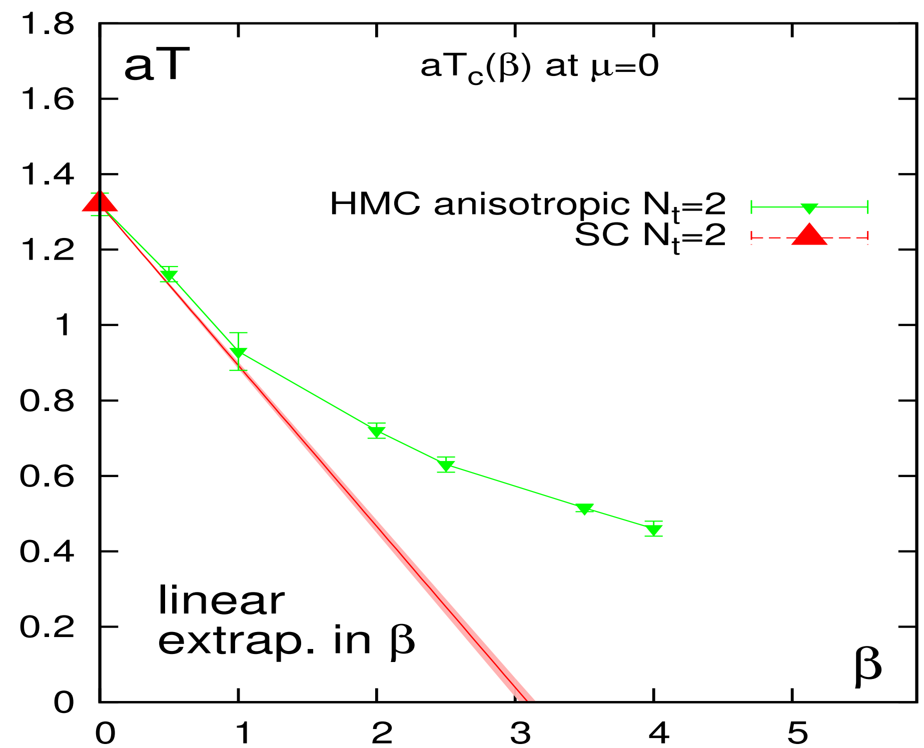
- Chiral transition ($m_q = 0$): 2nd $\to$ 1rst order as μ increases: *tricritical* point
- finite-N_t corrections $\to$ continuous-time. (then, no re-entrance)
- Polyakov $\neq$ anti-Polyakov loop. Both "feel" chiral transition.

Toward the continuum limit at $\mathcal{O}(\beta)$ 1406.4397 $\rightarrow$ PRL

- Introduce auxiliary plaquette variables $q_P = \{0,1\}$:

$$\exp(\frac{\beta}{N_c}\mathrm{ReTr}\ U_P) = \sum_{q_P=\{0,1\}} \left(\delta_{q_P,0} + \delta_{q_P,1}\frac{\beta}{N_c}\mathrm{ReTr}U_P\right) + \mathcal{O}(\beta^2)$$

- Sample $\{q_P\}$ $\rightarrow$ exact at $\mathcal{O}(\beta)$
- $q_P = 1 \rightarrow$ new color-singlet hopping terms qqg, $\bar{q}g$, from $\int dU U e^{-(\bar{\psi}U\psi - h.c.)}$:
  - hadrons acquire *structure*
  - hadron interaction by *gluon exchange*



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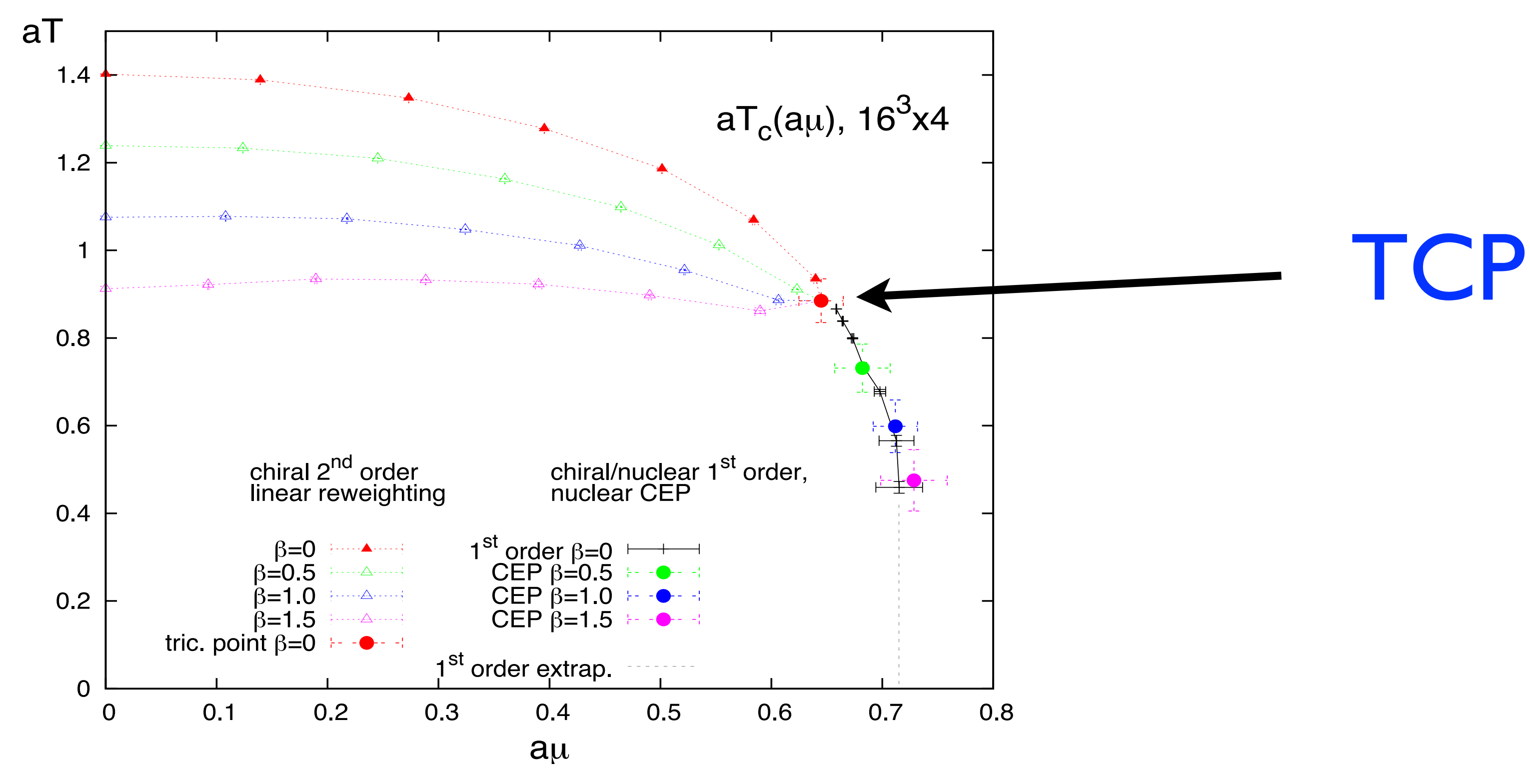

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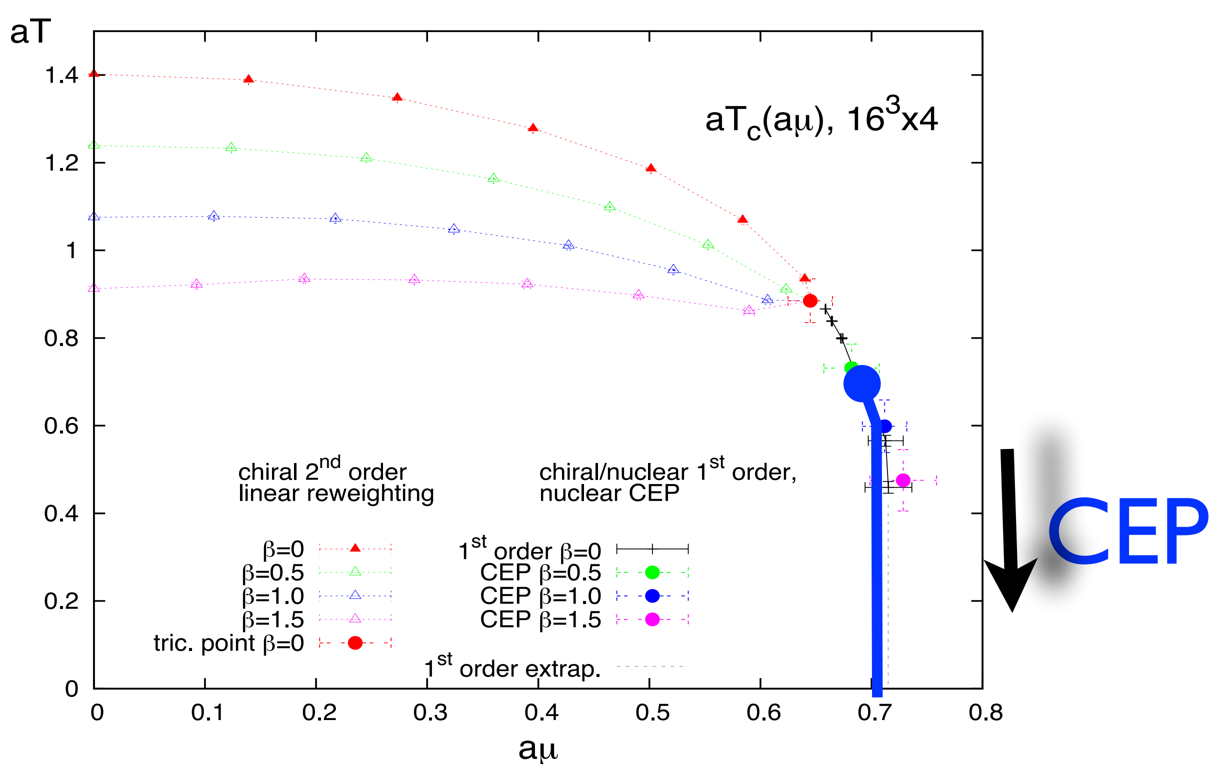

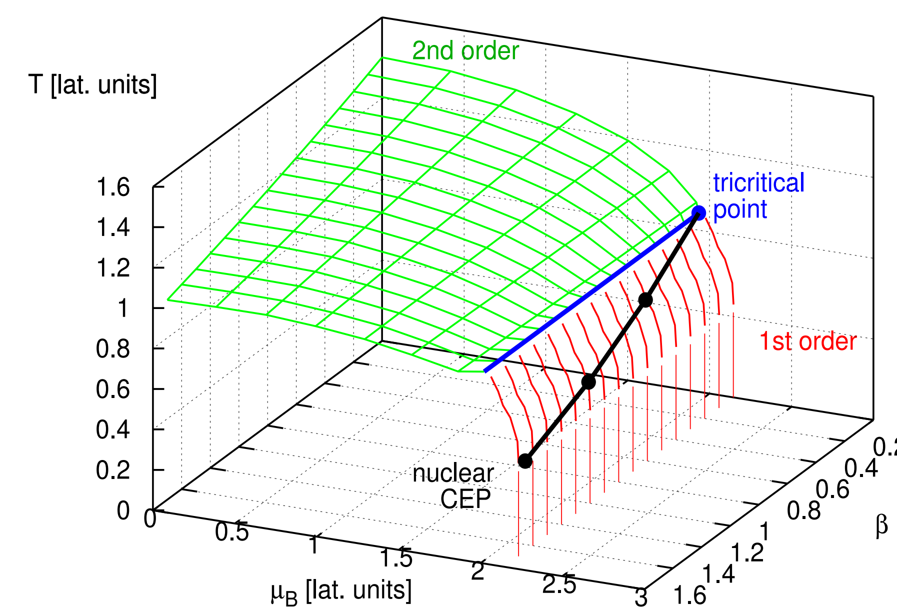

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  - liquid-gas CEP splits and moves down ?

Going beyond $\mathcal{O}(\beta)$ Vairinhos & PdF, 1409.8442

- $\beta = 0$: gauge links U are not directly coupled to each other:

$$Z(\beta = 0) = \int \prod_x d\bar{\psi} d\psi \quad \prod_{x,\nu} \left(\int dU_{x,\nu} e^{-\{\bar{\psi}_x U_{x,\nu} \psi_{x+\hat{\nu}} - h.c.\}} \right)$$

Product of 1-link integrals performed analytically

- $\beta \neq 0$: Plaquette 4-link coupling prevents analytic integration of gauge links

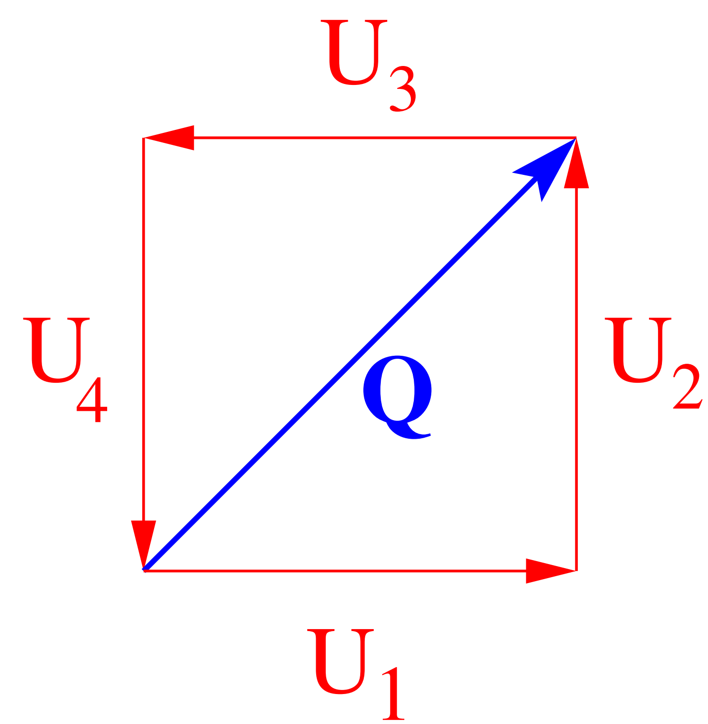
Decouple gauge links by Hubbard-Stratonovich transformation:

Hubbard-Stratonovich variant:

$$\beta \ \mathrm{ReTr} U_P$$

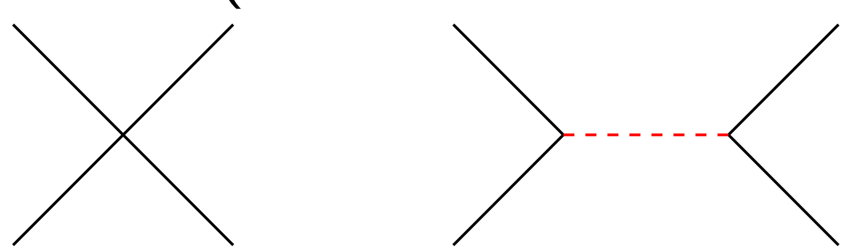
$$\Updownarrow$$

$$-\beta \ \mathrm{ReTr} \left(|Q|^2 - Q^\dagger U_1 U_2 - U_3 U_4 Q \right)$$



ie. "2-link" action (Fabricius & Haan, 1984)

Cf. 4-fermi



Further decoupling to "1-link" action $\rightarrow$ link integration possible $\forall \beta$

2-link action $\to$ 1-link $\to$ 0-link

Vairinhos & PdF, 1409.8442

- Hubbard-Stratonovich: $\forall Y \in \mathbf{C}^{N\times N}$, $\quad e^{\mathrm{Tr} Y^\dagger Y} = \mathcal{N} \int dX \; e^{\mathrm{Tr}(X^\dagger Y + X Y^\dagger)}$

where $X \in \mathbf{C}^{N\times N}$ with Gaussian measure $dX \propto \prod_{ij} dx_{ij} dx_{ij}^* e^{-|x_{ij}|^2}$

2-link action → 1-link → 0-link

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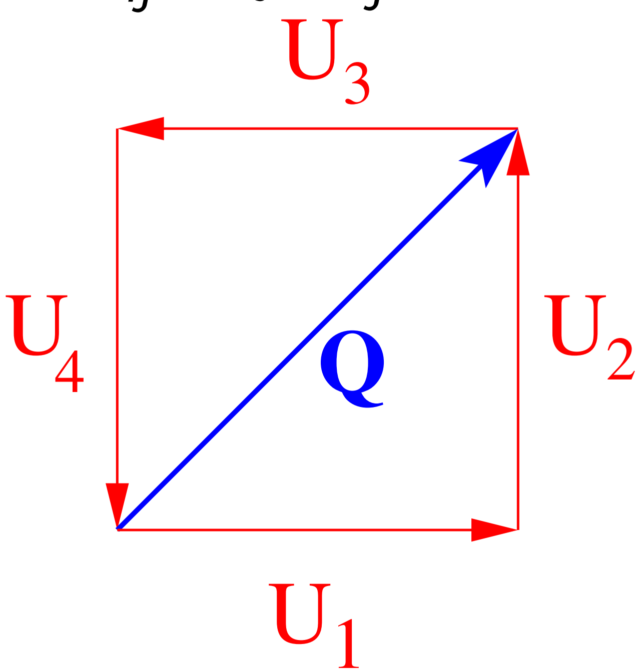
- 4 → 2-link action:

$Y = (U_1 U_2 + U_4^\dagger U_3^\dagger)$, $X = Q$

$$S_{2-\mathrm{link}} = \mathrm{ReTr}\ Q^\dagger (U_1 U_2 + U_4^\dagger U_3^\dagger)$$



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Vairinhos & PdF, 1409.8442

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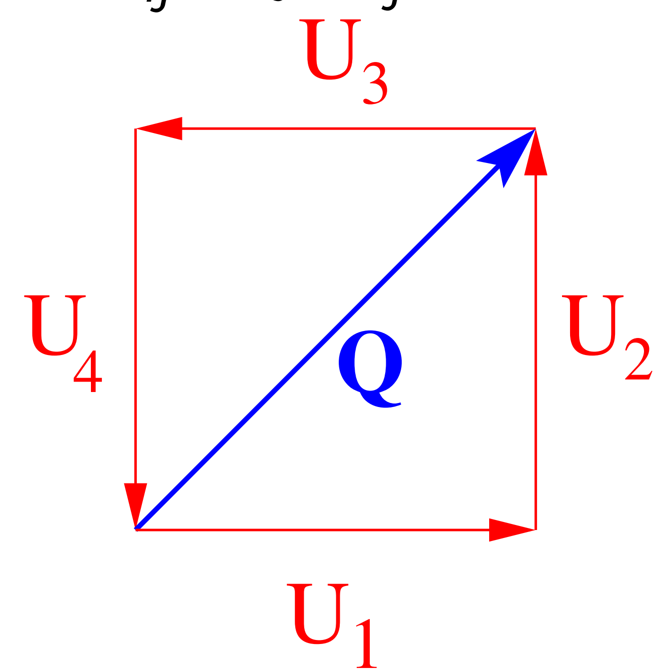
where $X \in \mathbf{C}^{N\times N}$ with Gaussian measure $dX \propto \prod_{ij} dx_{ij} dx^*_{ij} e^{-|x_{ij}|^2}$

- 4 → 2-link action:

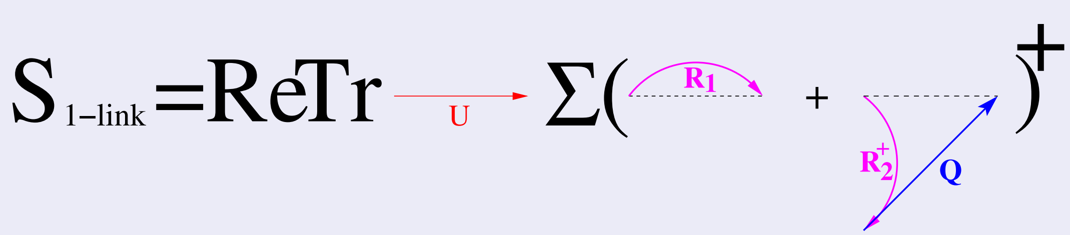
$$Y = (U_1 U_2 + U_4^\dagger U_3^\dagger),\ X = Q$$

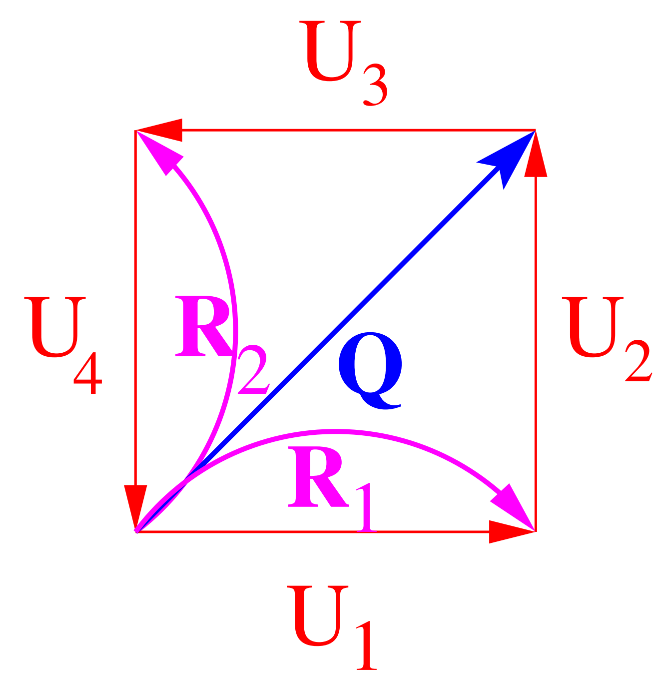
$$S_{2-\mathrm{link}} = \mathrm{ReTr}\ Q^\dagger (U_1 U_2 + U_4^\dagger U_3^\dagger)$$



- 2 → 1-link action:

$$Y = (U_1 + Q U_2^\dagger),\ X = R_1$$





2-link action $\rightarrow$ 1-link $\rightarrow$ 0-link

Vairinhos & PdF, 1409.8442

- Hubbard-Stratonovich: $\forall Y \in \mathbf{C}^{N\times N}$, $\quad e^{\mathrm{Tr} Y^\dagger Y} = \mathcal{N} \int dX \; e^{\mathrm{Tr}(X^\dagger Y + X Y^\dagger)}$

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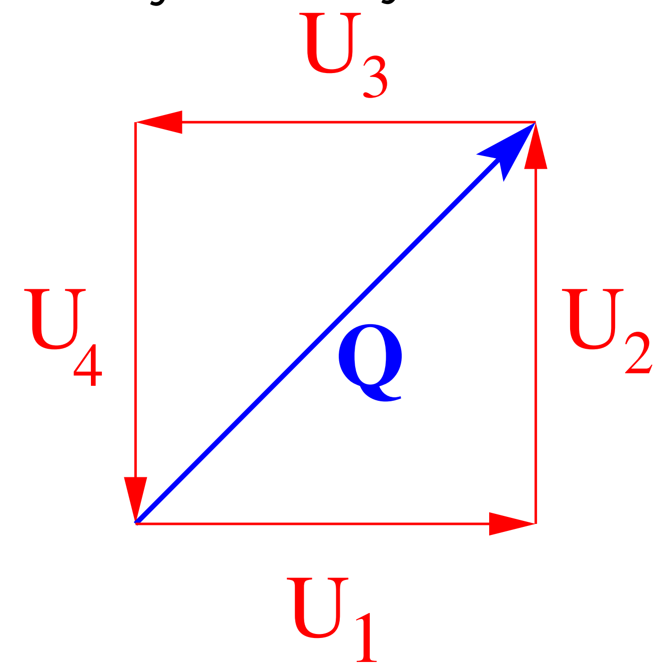
- $4 \rightarrow 2$-link action:

$$Y = (U_1 U_2 + U_4^\dagger U_3^\dagger),\; X = Q$$

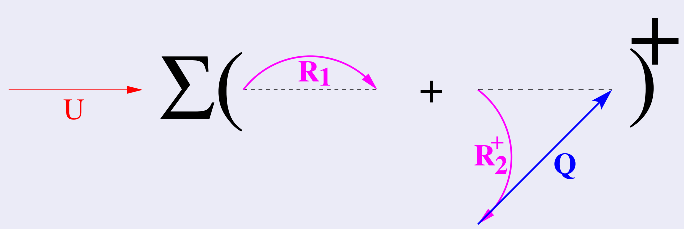
$$S_{2-\mathrm{link}} = \mathrm{ReTr}\; Q^\dagger (U_1 U_2 + U_4^\dagger U_3^\dagger)$$

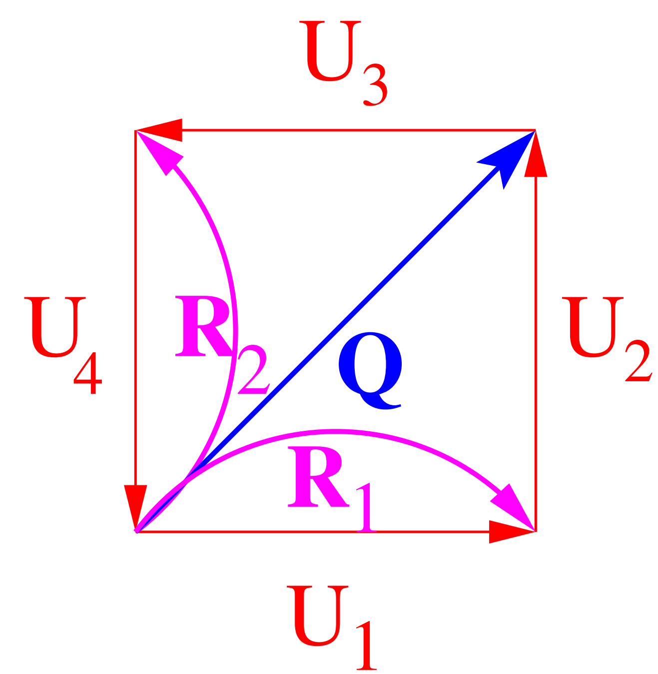


- $2 \rightarrow 1$-link action:

$$Y = (U_1 + Q U_2^\dagger),\; X = R_1$$

$S_{1-\mathrm{link}} = \mathrm{ReTr}$

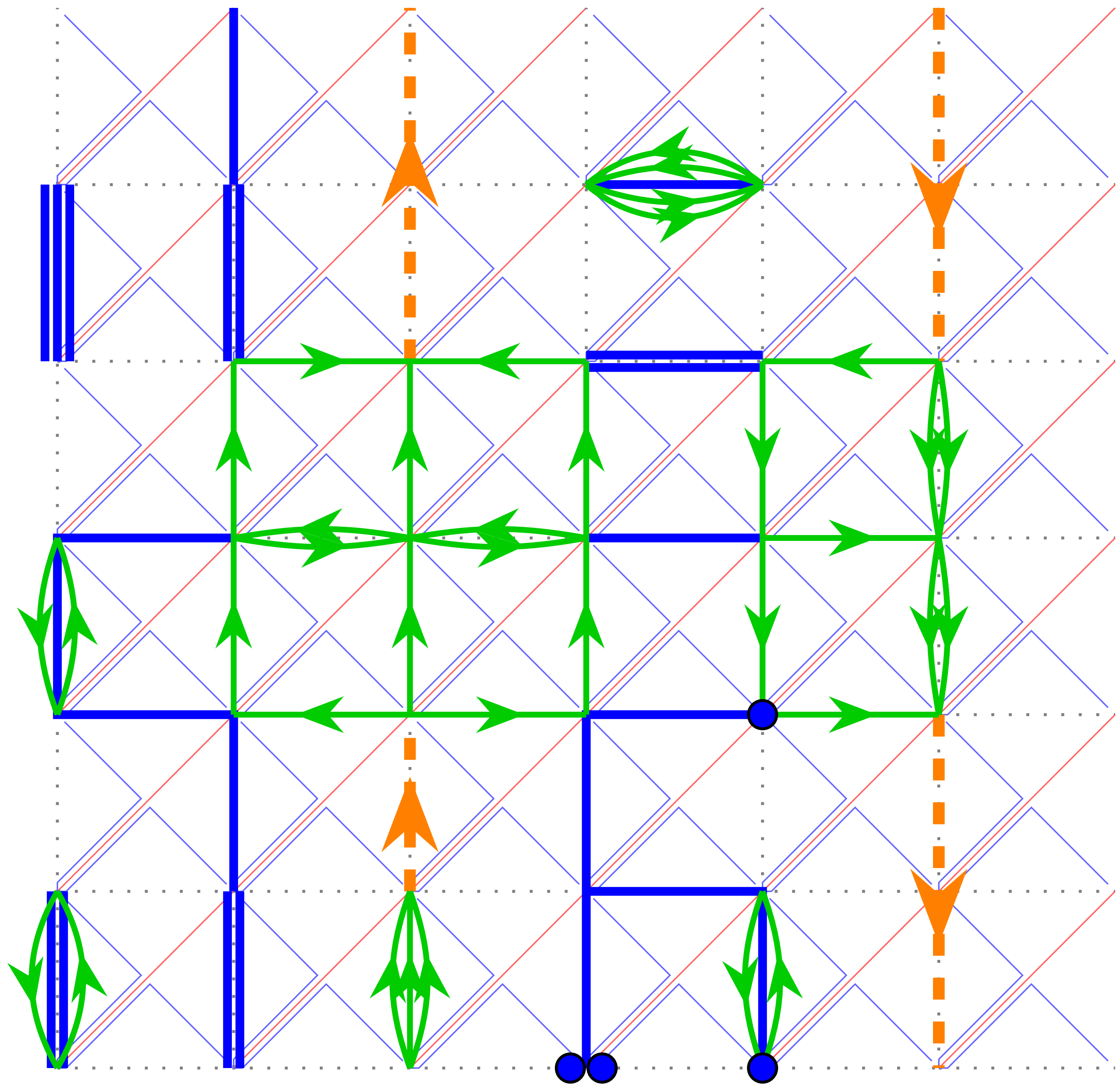




- $1 \rightarrow 0$-link action: integrate out U analytically – *also with fermion sources*

QCD with graphs

$\beta > 0 \;\rightarrow\;$ Monomers, dimers, baryons, *quarks*, all in the background of $\{Q, R\}$



Start with a simpler case: 2*d* QED

- Extend 0-link representation of 2*d* $U(1)$ with staggered fermions:

$$Z(\beta,m) = \int \left[\prod_x d\chi_x d\bar{\chi}_x e^{2am\bar{\psi}_x\psi_x}\right] \int \mathcal{G}_\beta[Q,R] \prod_{x,\mu} \int dU\, e^{\mathrm{Re}\left(\left(\beta J^\dagger_{x\mu} + 2\eta_{x\mu}\psi_x\psi_{x+\hat{\mu}}\right)^\dagger U\right)}$$

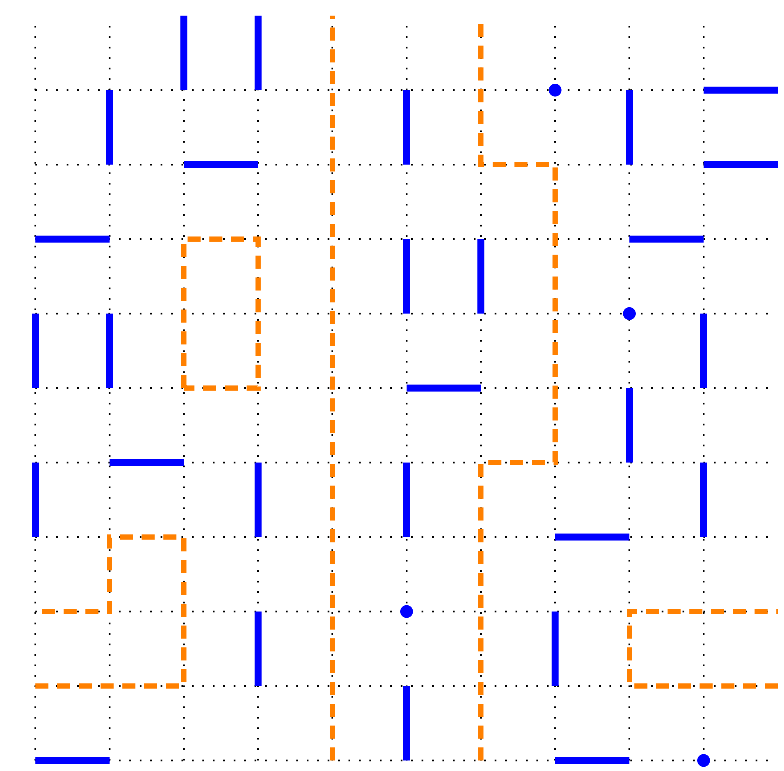
$$= \int \mathcal{G}_\beta[Q,R] \prod_{x,\mu} I_0(\beta|J_{x\mu}|) \sum_{\{n,k,C\}} \left(\prod_x (2am)^{n_x}\right)\left(\sigma_F(C) \prod_{i=1}^{\#C} 2\,\mathrm{Re}(W(C))\right)$$

i.e. monomers, dimers and electron loops

- weight of electron loop is *global* and can be *negative*

$$W(C) = \prod_{(x,\mu)\in C} \widetilde{U}_{x\mu}$$

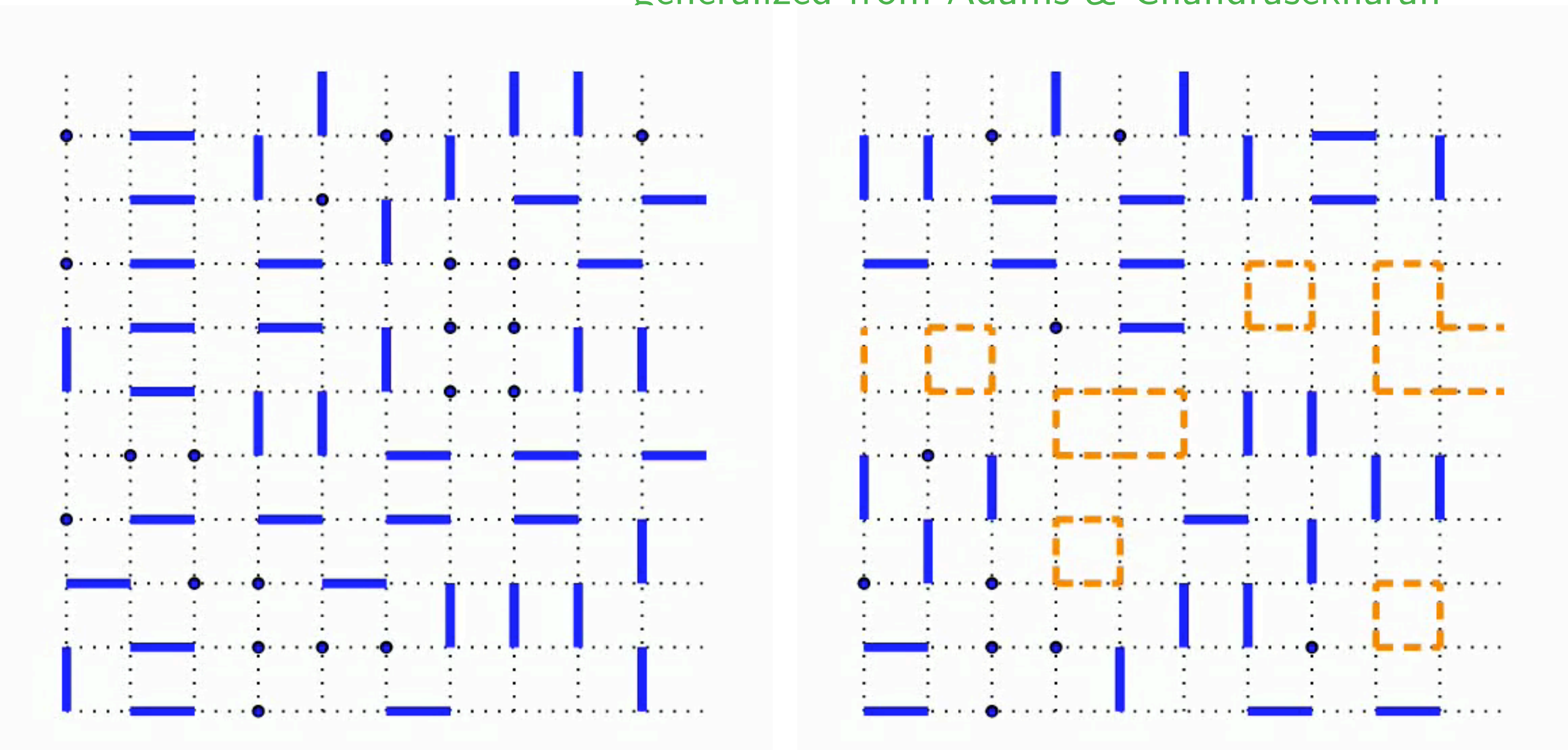
$$\widetilde{U}_{x\mu} = \frac{I_1(\beta|J_{x\mu}|)}{I_0(\beta|J_{x\mu}|)} \frac{J_{x\mu}}{|J_{x\mu}|}$$



Monte Carlo

- Gaussian heatbath to update $\{Q, R\}$
- "Meson" worm to update monomers and dimers
- "Electron" worm to update electron loops and dimers

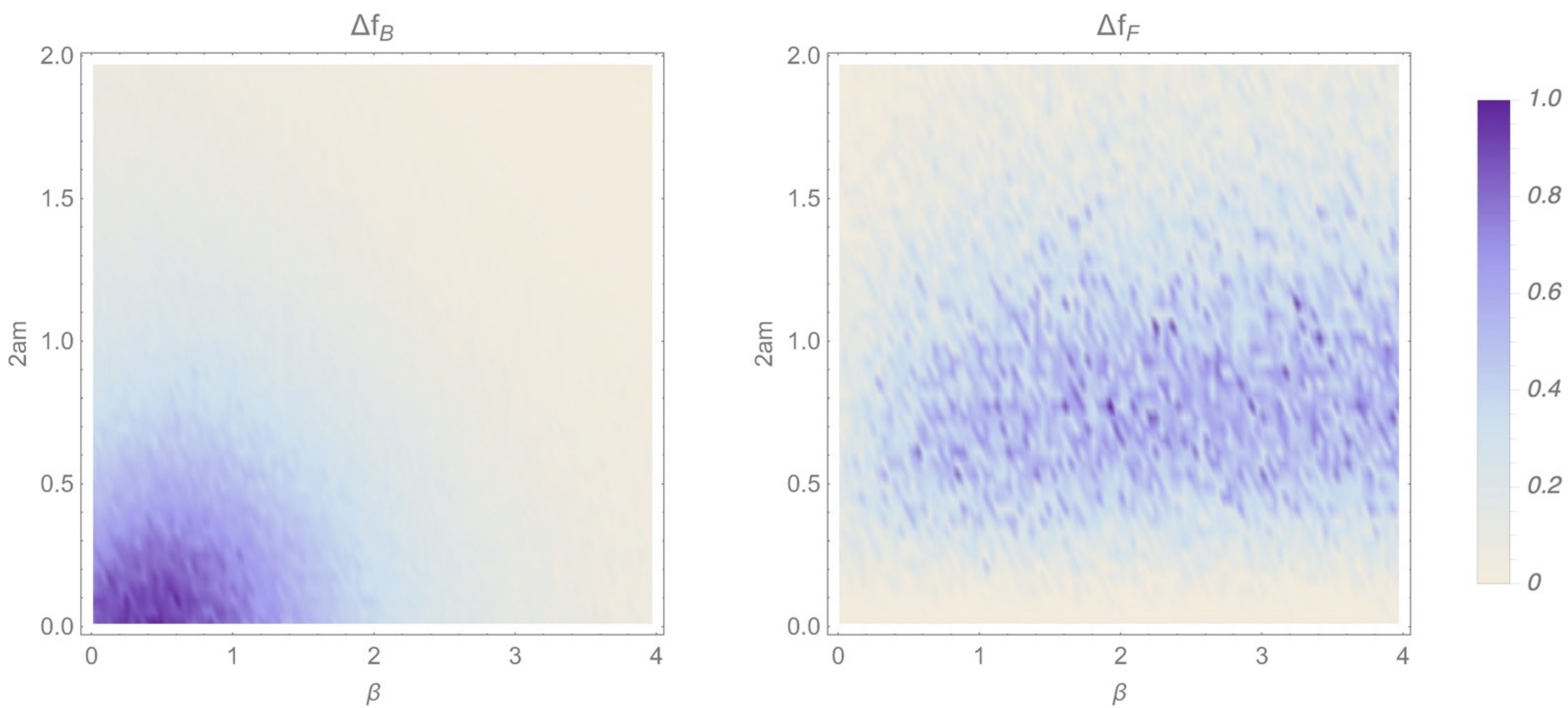
generalized from Adams & Chandrasekharan



Sign problems

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

$$\sigma(C) = \underbrace{\mathrm{sign}\left(\prod_{i=1}^{\#C} 2\,\mathrm{Re}(W(C_i))\right)}_{\sigma_B(C)} \times \sigma_F(C)$$



Conclusions

- Tolstoi:

"Happy families are all alike; each unhappy family is unhappy in its own way"

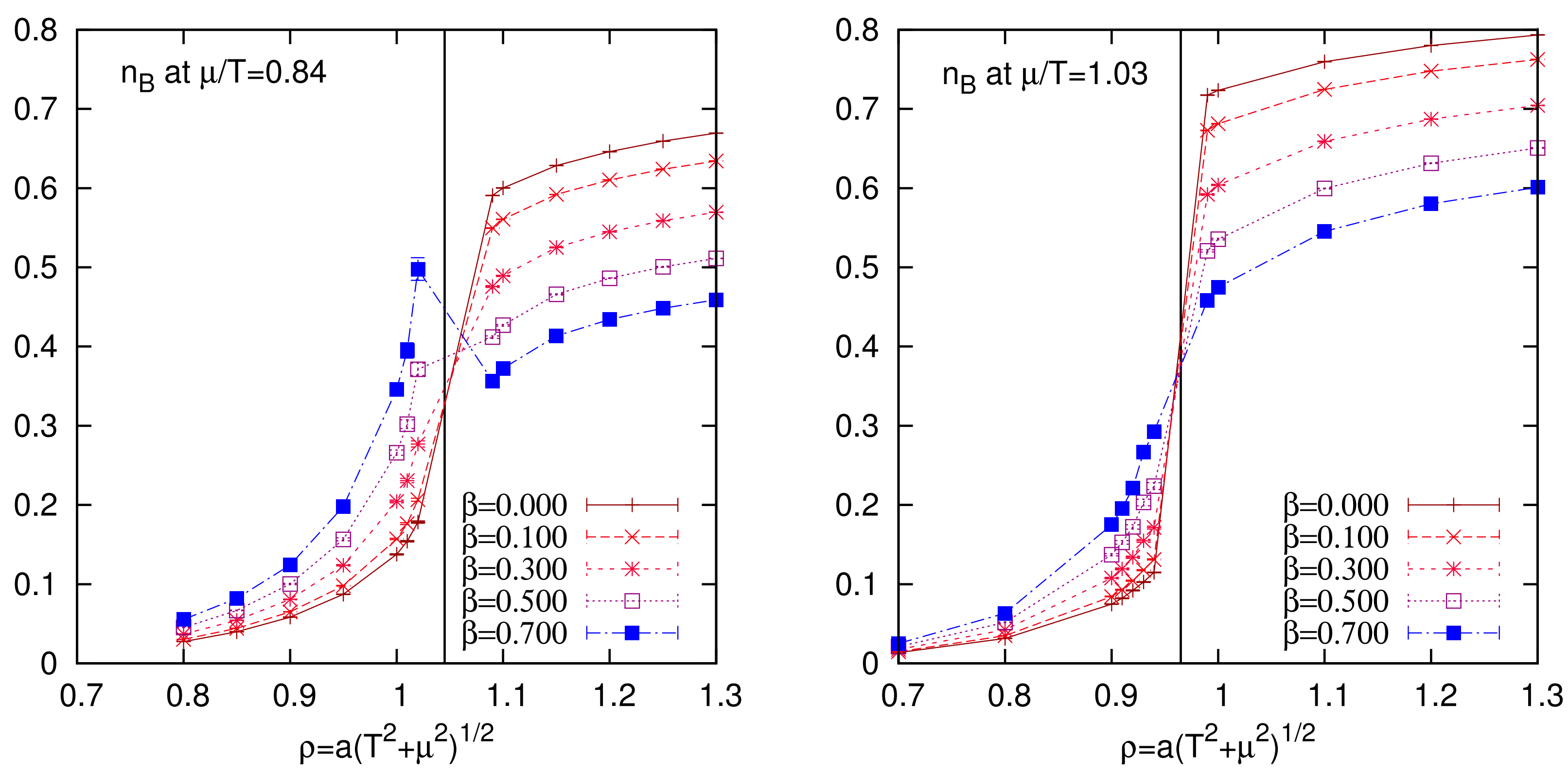
"happy" $\longrightarrow$ sign-pb free

- Finite-density QCD: still a long way to go...

Thank you for your attention

Backup

Liquid-gas endpoint moves to lower temperatures as β increases



Jump at $\beta = 0$ becomes crossover as β grows

Monte Carlo algorithms

- **Bosonic updates:**
  1. **Gaussian heatbath** for the auxiliary fields (Q, R) + HS transformations (with the help of an auxiliary $U(1)$ field)
  2. Metropolis update to correct for electron loop weights

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

- **Fermionic updates:**
  1. **"Meson" worm algorithm:** Updates the monomer-dimer cover, with target distribution:

$$w_m = \prod_x (2am)^{n_x} \prod_{x,\mu} 1$$

  2. **Electron worm algorithm:** Transforms electron loops into dimers and vice versa, with target distribution:

$$w_e = \prod_{x,\mu} 1 \prod_{i=1}^{\#C} |2\mathrm{Re}(W(C_i))| = \underbrace{\prod_{x,\mu} 1 \left(\frac{I_1(\beta|J_{x\mu}|)}{I_0(\beta|J_{x\mu}|)}\right)^{b_{x\mu}}}_{\text{Worm (local)}} \underbrace{\prod_{i=1}^{\#C} |2\cos(\varphi(C_i))|}_{\text{Metropolis (global)}}$$

Adams & Chandrasekharan (2003)

Chandrasekharan & Jiang (2006)