Progress in the simulation of QCD at non-zero baryon density

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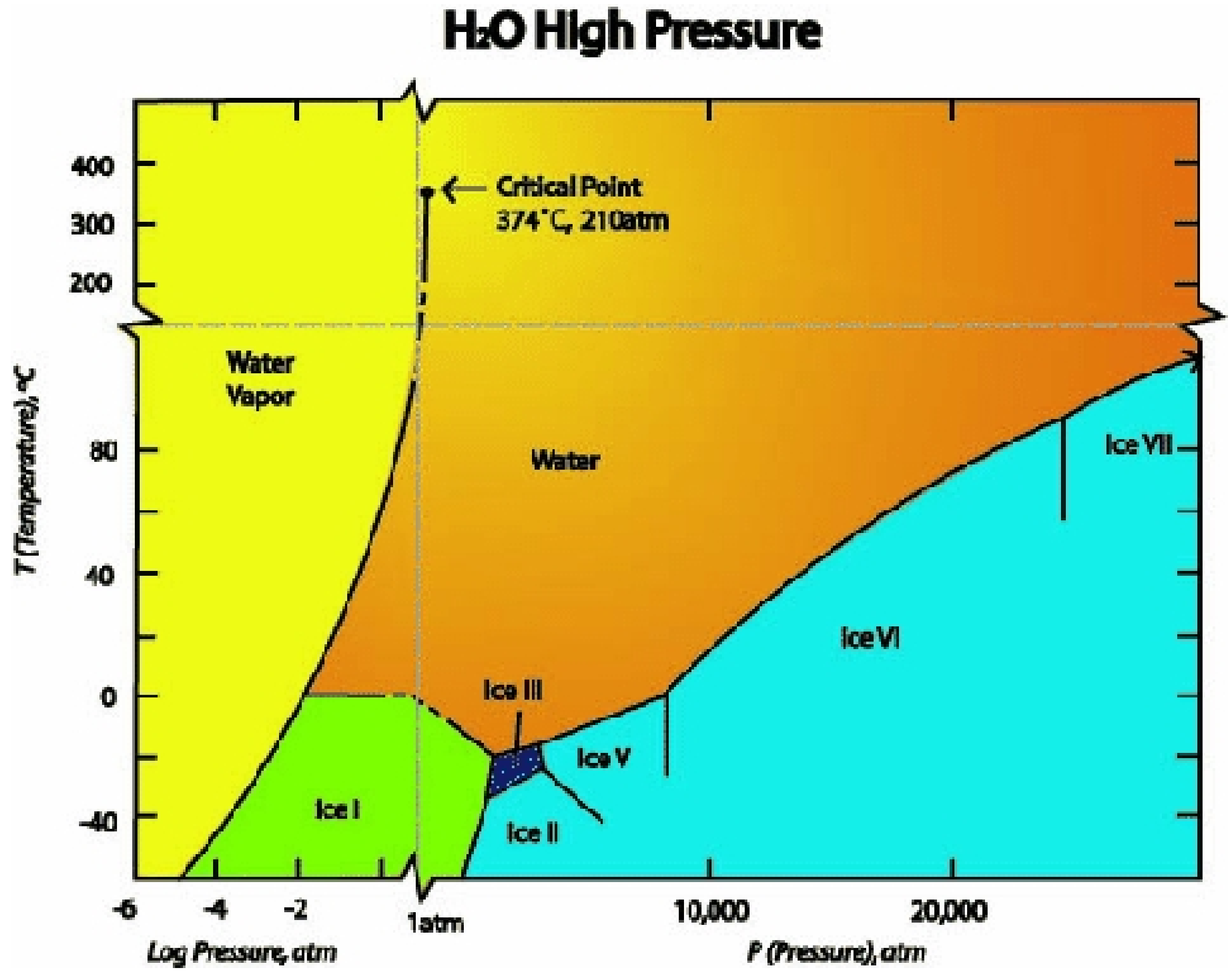
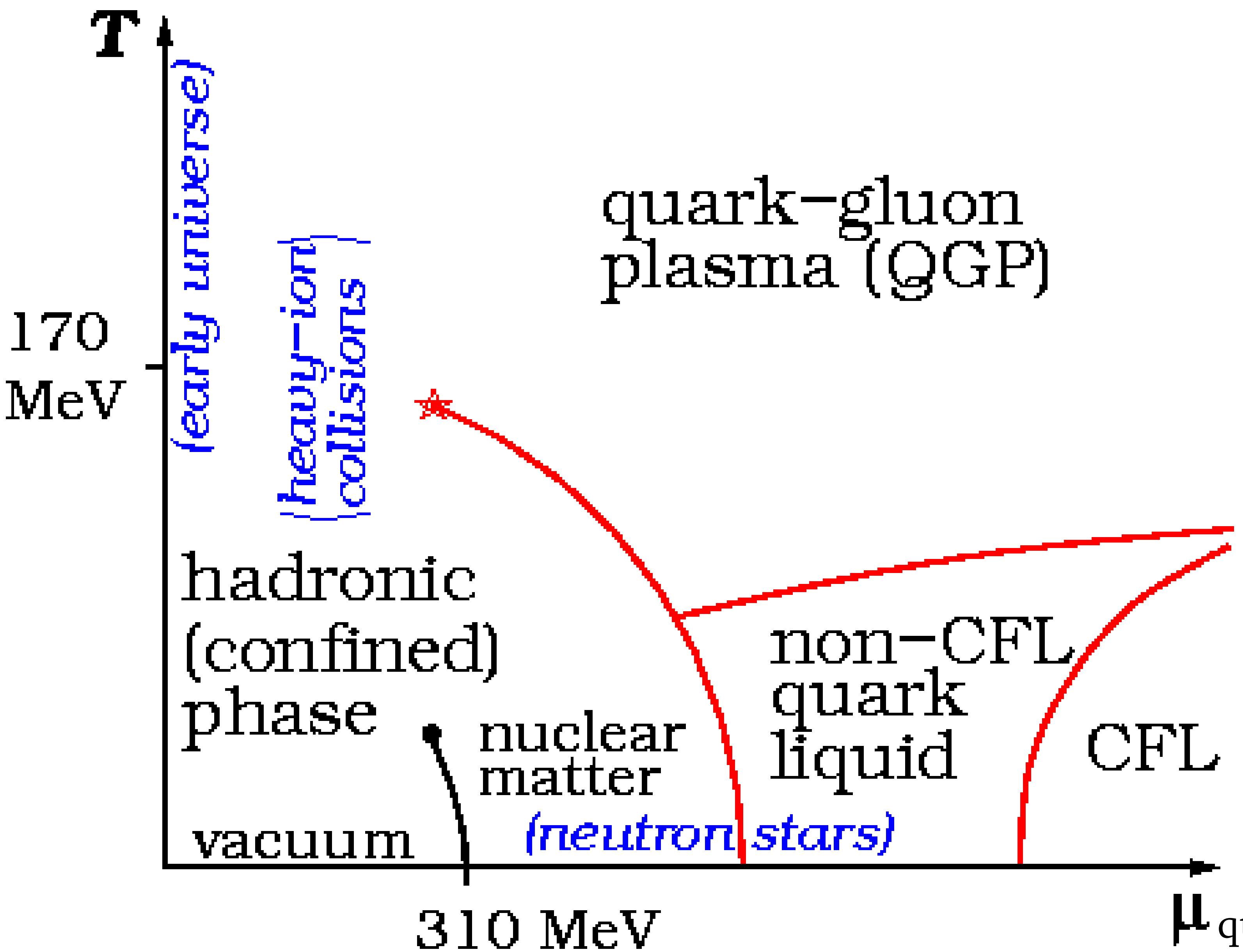
Water changes its state when heated or compressed



What happens to quarks and gluons when heated or compressed?

The phase diagram of QCD according to Wikipedia



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

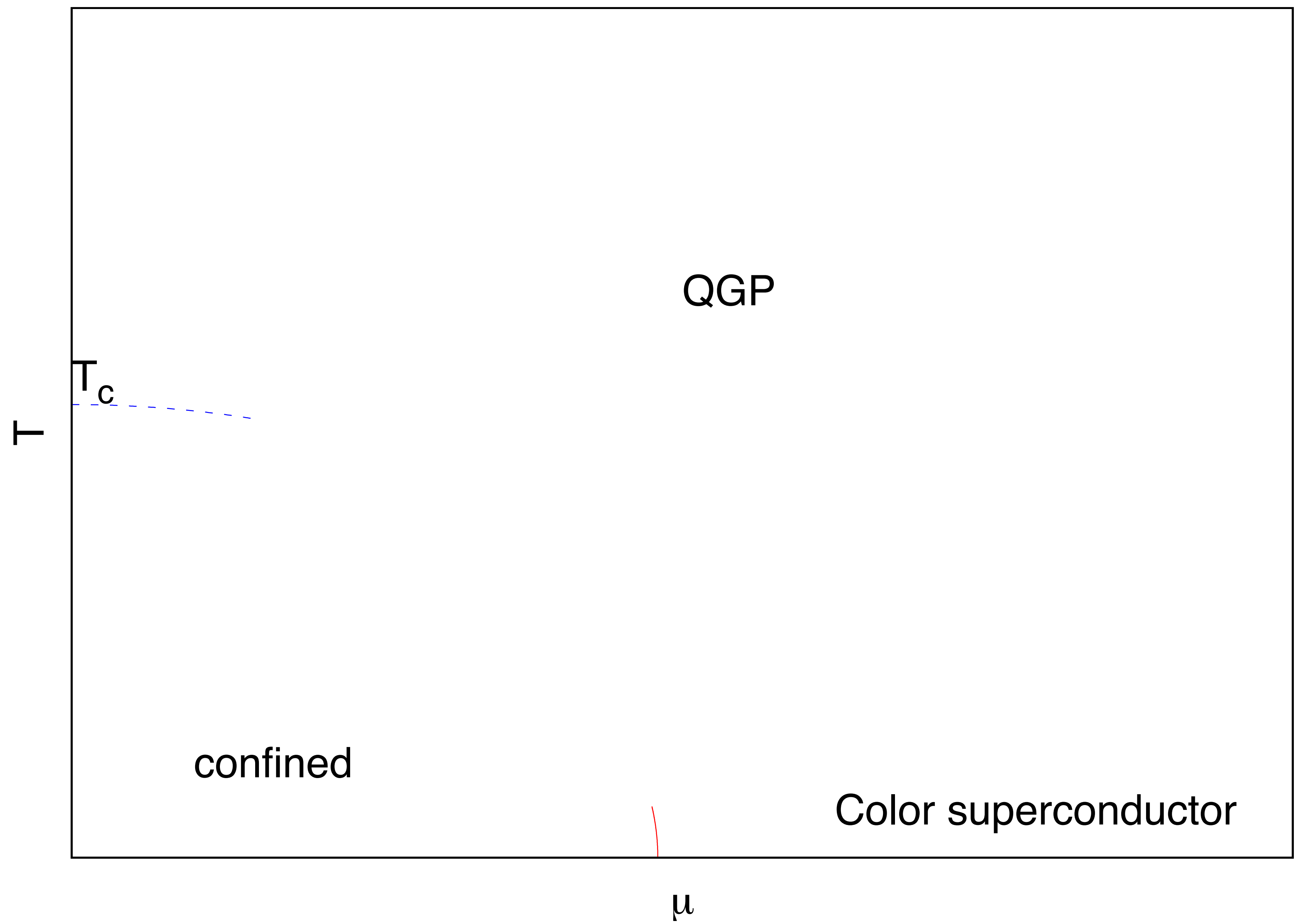
Also ?

- crystal phase(s)
- quarkyonic phase
- strangelets

...

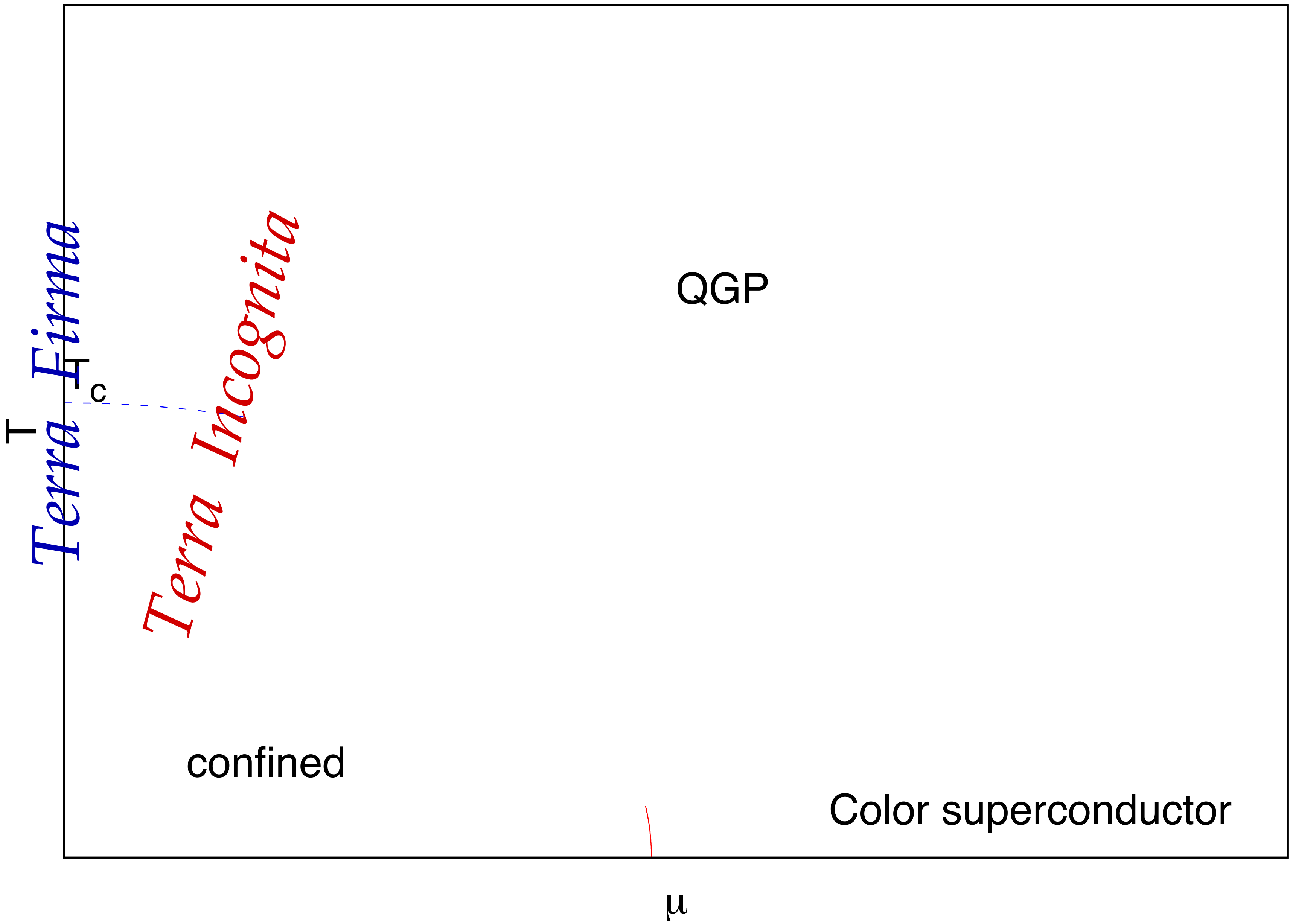
Everything in red is a conjecture

Finite μ: what is known?



Minimal, possible phase diagram

Finite μ: what is known?



Exploration hampered by sign problem

Why are we stuck at $\mu = 0$? The "sign problem"

- quarks anti-commute $\rightarrow$ integrate analytically: $\det(\not{D}(U) + m + \mu\gamma_0)$
  $\gamma_5(i\not{p} + m + \mu\gamma_0)\gamma_5 = (-i\not{p} + m - \mu\gamma_0) = (i\not{p} + m - \mu^*\gamma_0)^\dagger$

$$\det \not{D}(\mu) = \det{}^* \not{D}(-\mu^*)$$

det real only if $\mu = 0$ (or $i\mu_i$), otherwise can/will be complex

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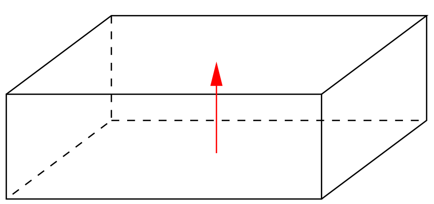
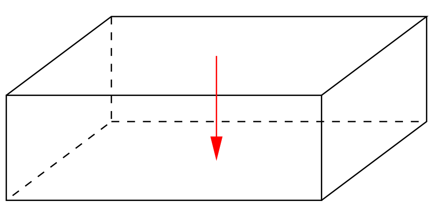
- Measure $d\varpi \sim \det \not{D}$ *must be complex* to get correct physics:



$$\langle \mathrm{Tr\ Polyakov} \rangle = \exp(-\tfrac{1}{T}F_{\mathbf{q}}) = \int \mathrm{Re\ Pol} \times \mathrm{Re}\ d\varpi - \mathrm{Im\ Pol} \times \mathrm{Im}\ d\varpi$$



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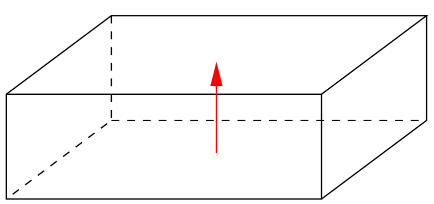

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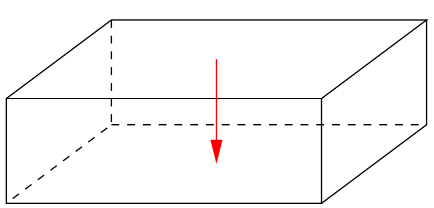

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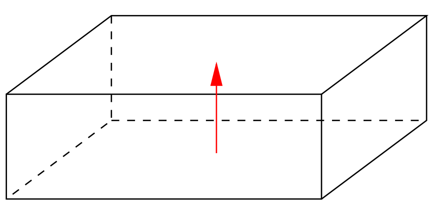

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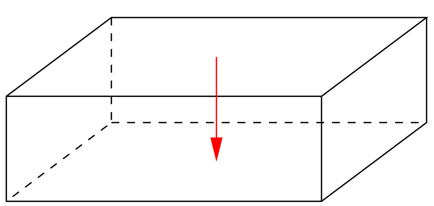

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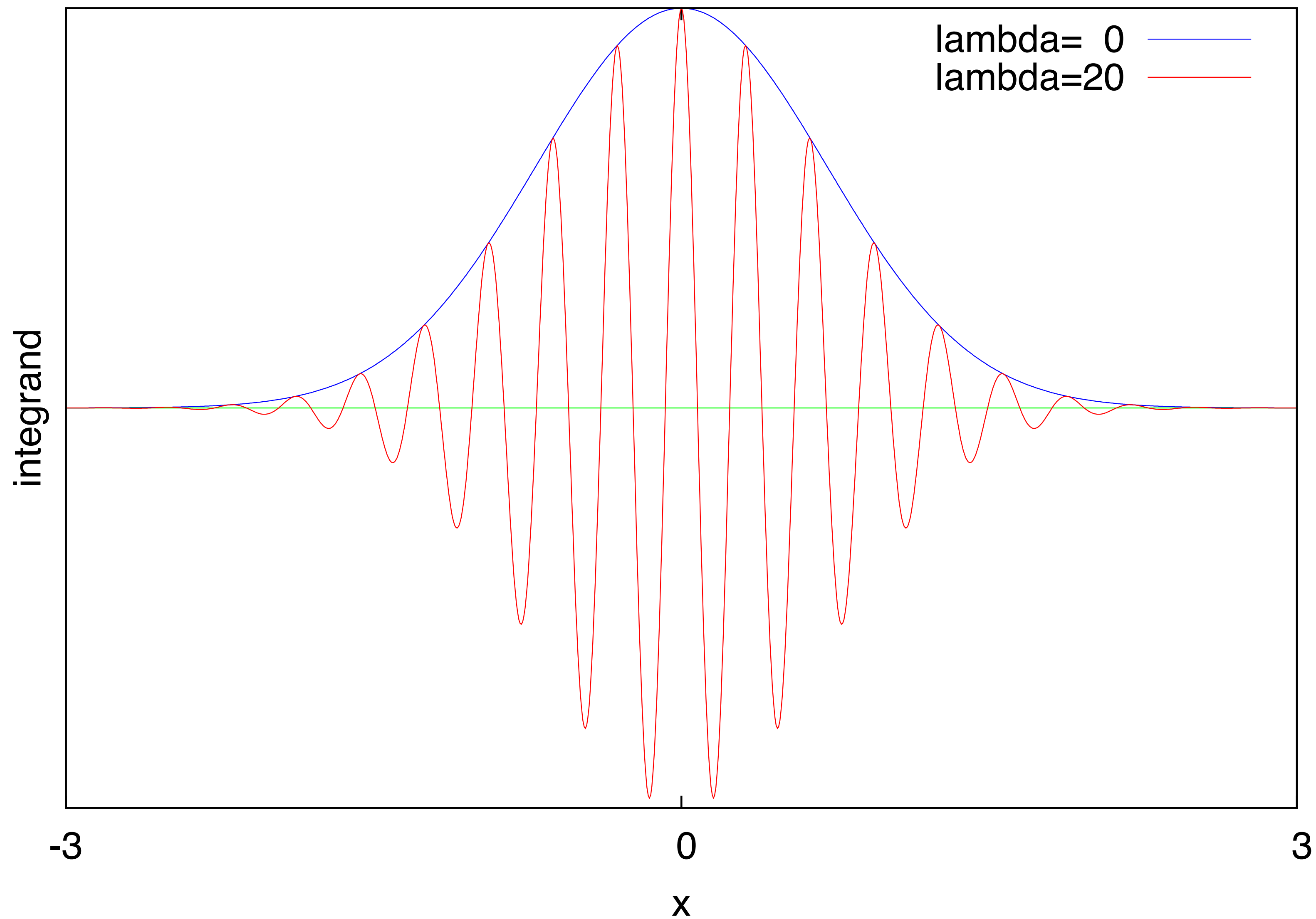
Complex determinant $\Longrightarrow$ no probabilistic interpretation $\longrightarrow$ Monte Carlo ??

Sampling oscillatory integrands

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



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

Reweighting

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

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

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

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

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

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

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

$$\boxed{\Delta f \text{ measures severity of sign pb.}}$$

Sampling for QCD at finite μ

- QCD: sample with $|\mathrm{Re}(\det(\mu)^{N_f})|$ optimal, but not equiv. to Gaussian integral
  Can choose instead: $|\det(\mu)|^{N_f}$, i.e. "phase quenched"
  $|\det(\mu)|^{N_f} = \det(+\mu)^{\frac{N_f}{2}} \det(-\mu)^{\frac{N_f}{2}}$, ie. isospin chemical potential $\mu_u = -\mu_d$
  couples to $u\bar{d}$ charged pions $\Rightarrow$ Bose condensation of π^+ when $|\mu| > \mu_{\mathrm{crit}}(T)$

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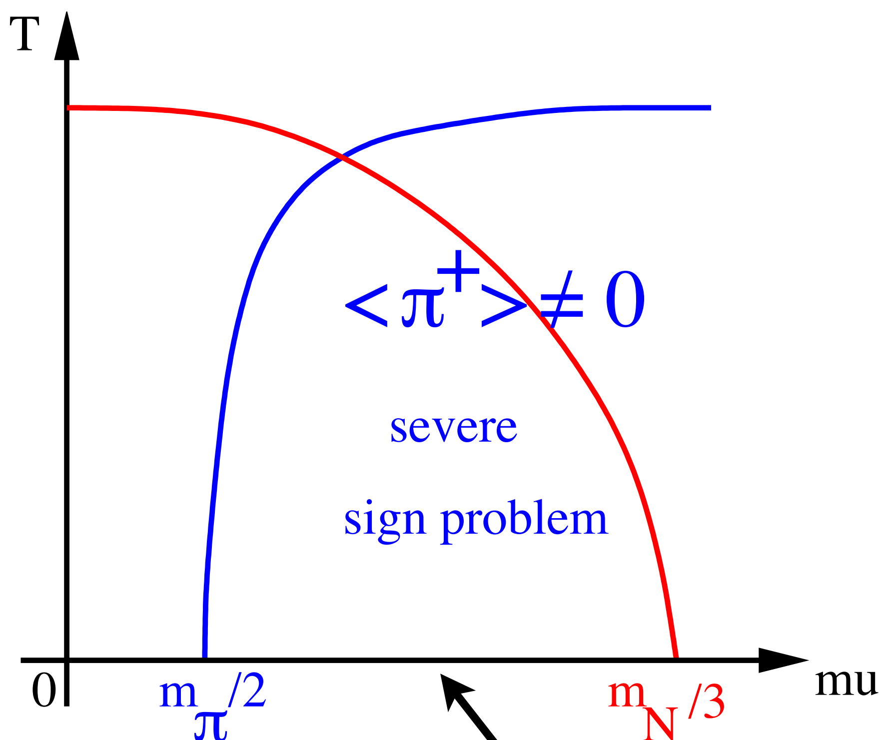
- av. sign $= \frac{Z_{\mathrm{QCD}}(\mu)}{Z_{|\mathrm{QCD}|}(\mu)} = e^{-\frac{V}{T}[f(\mu_u=+\mu,\mu_d=+\mu)-f(\mu_u=+\mu,\mu_d=-\mu)]}$ (for $N_f = 2$)



$\Delta f(\mu^2, T)$ large in the Bose phase
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"Silverblaze pb": phase of det changes groundstate

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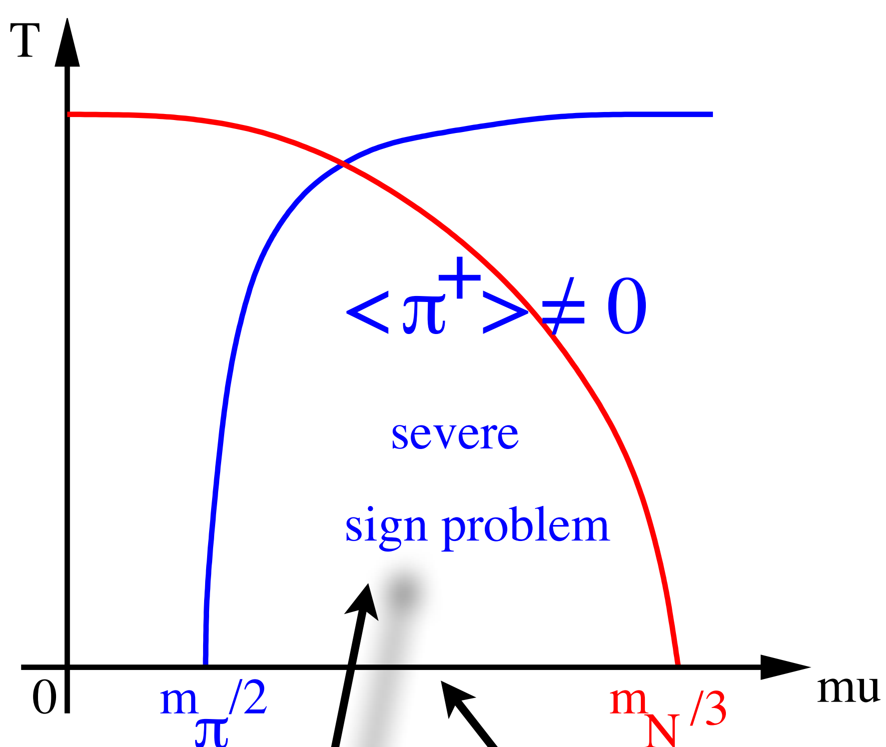

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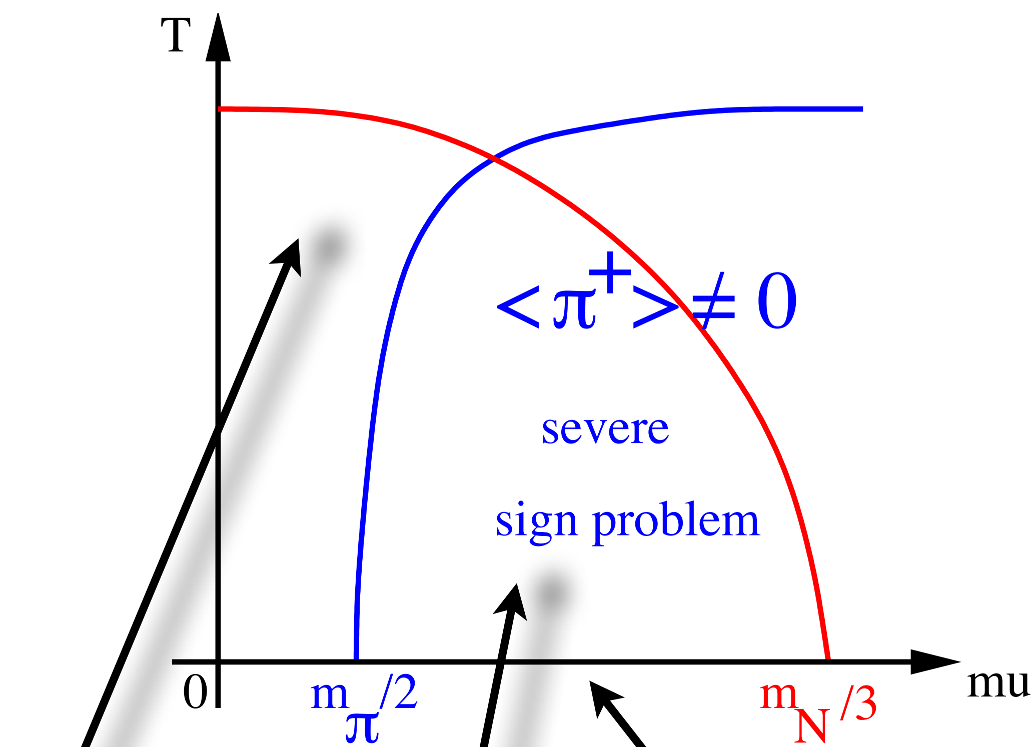

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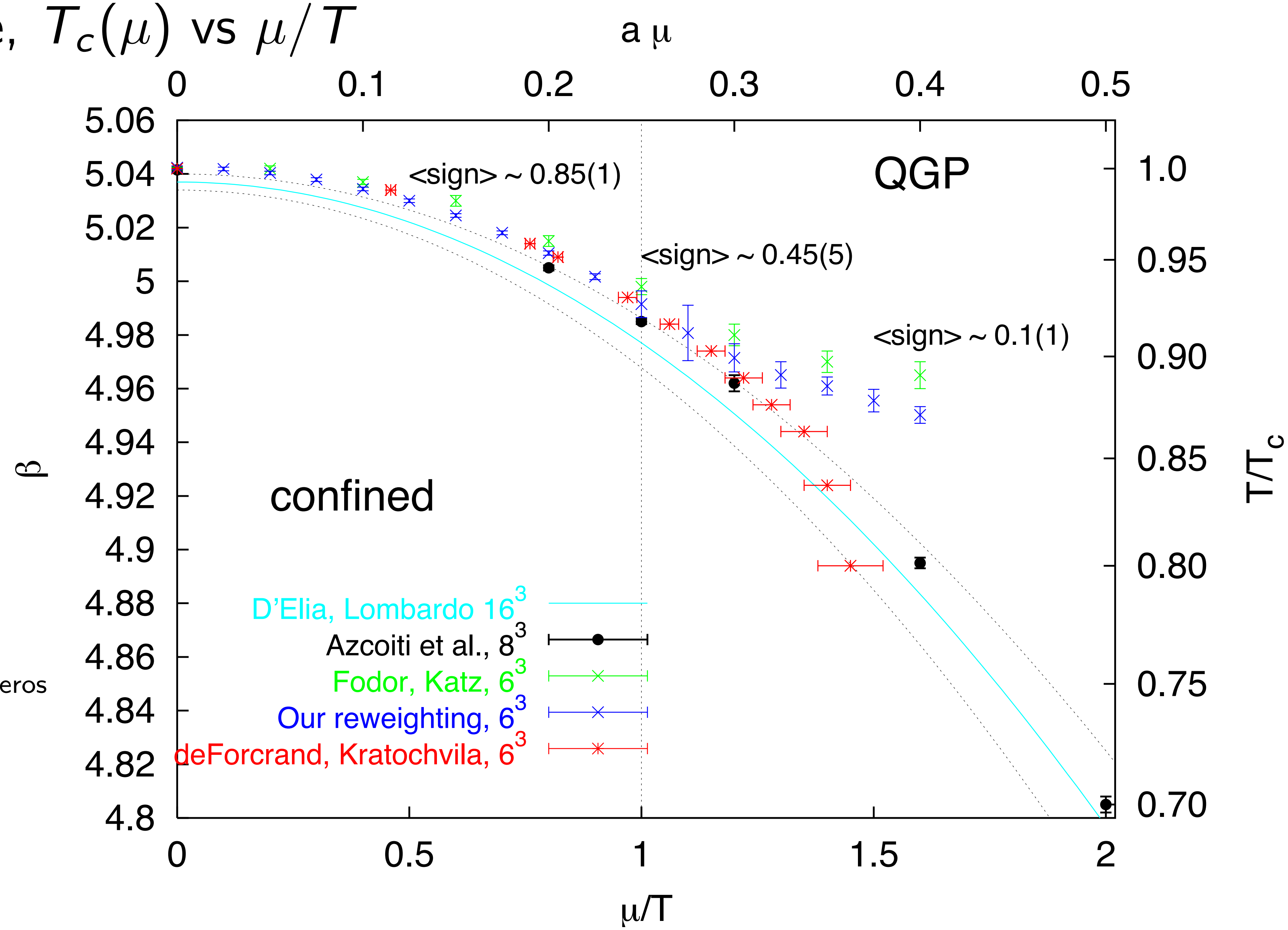
Not as hard
$\frac{\mu}{T} \lesssim 1$

Valuable crosschecks

All methods agree for $\mu/T \lesssim \mathcal{O}(1)$ on small lattices

Here, $T_c(\mu)$ vs μ/T



imaginary μ
2 param. imag. μ
dble reweighting, LY zeros
Same, susceptibilities
canonical

$N_f = 4$ staggered,
$am_q = 0.05$, $N_t = 4$
PdF & Kratochvila
LAT05

- **Main results**: - curvature of pseudocritical line $\frac{d^2 T_c}{d\mu^2}|_{\mu=0}$
  - absence of critical point for $\frac{\mu}{T} \lesssim 1$

$\mu/T \gtrsim \mathcal{O}(1)$: 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 $\rightarrow \det(\{U\})$
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Reverse order:
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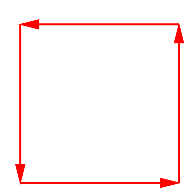
- Caveat: must turn off 4-link coupling  in $\beta\sum_P \mathrm{ReTr}U_P$ by setting $\beta = 0$

$\beta = 0$: 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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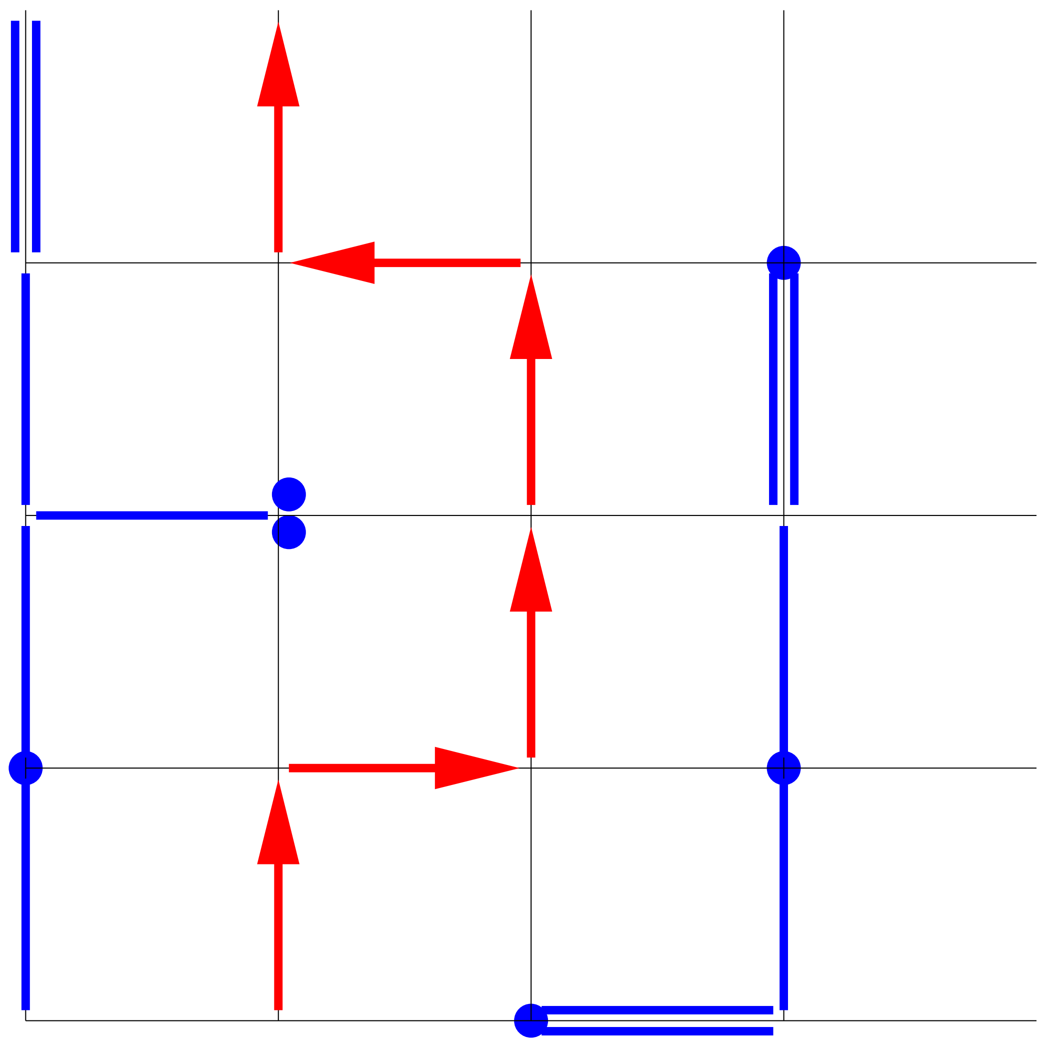

Constraint at every site:
3 blue symbols (• $\bar{\psi}\psi$, meson hop)
or a baryon loop

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

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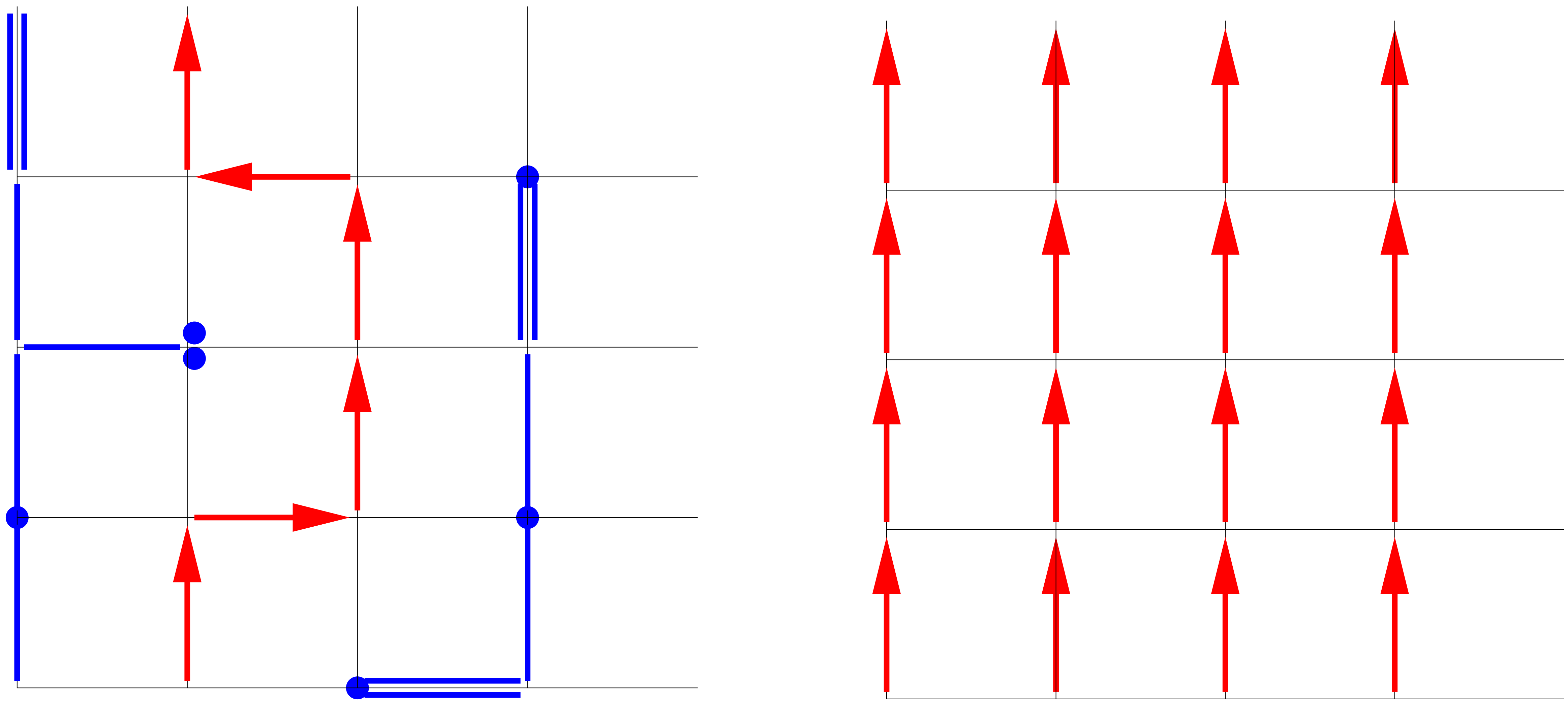

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The dense (crystalline) phase:
1 baryon per site; no space left
$\rightarrow \langle\bar{\psi}\psi\rangle = 0$

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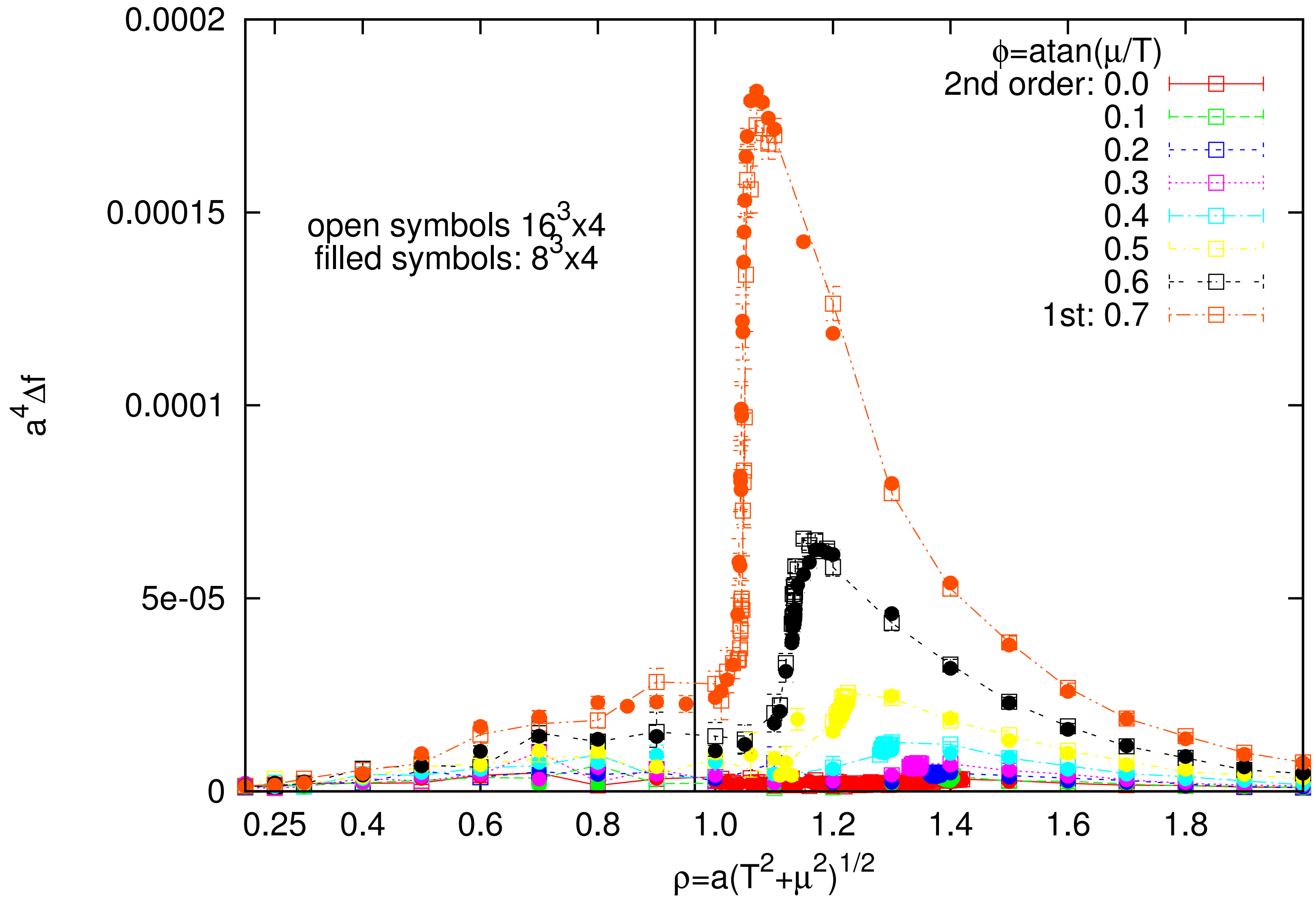
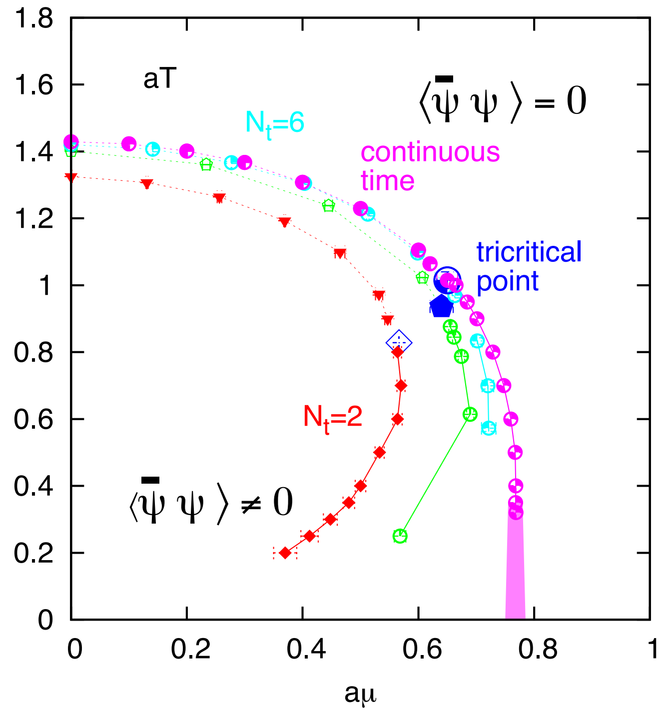
Sign problem? Monitor $-\frac{1}{V}\log\langle\text{sign}\rangle$

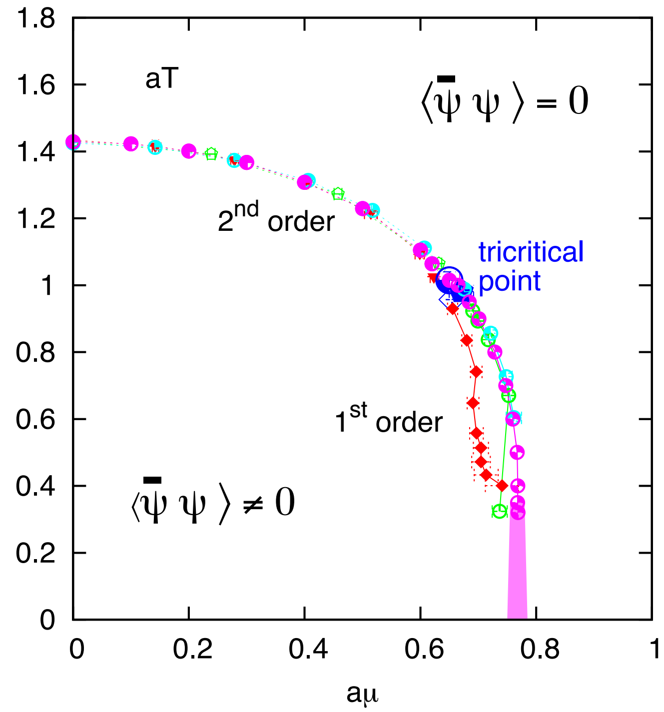


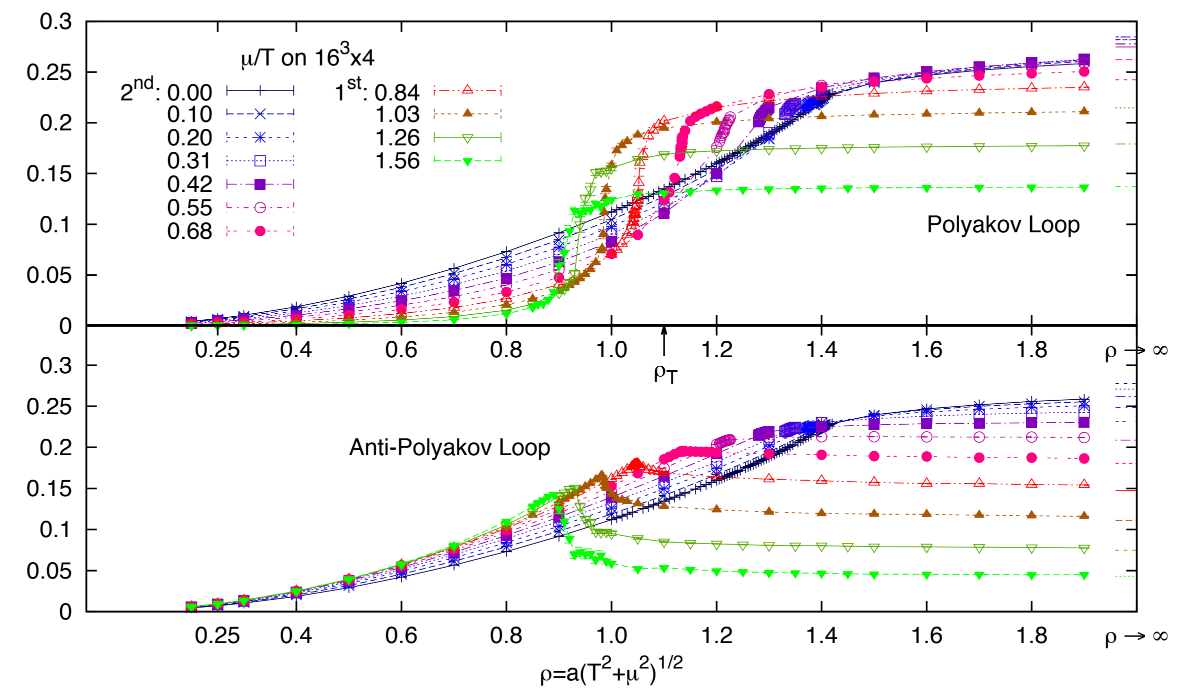
- $\langle\text{sign}\rangle = \frac{Z}{Z_{||}} \sim \exp(-\frac{V}{T}\Delta f(\mu^2))$ as expected
- Determinant method $\rightarrow \Delta f \sim \mathcal{O}(1)$. Here, **Gain $\mathcal{O}(10^4)$ in the exponent!**
  - heuristic argument correct: color singlets closer to eigenbasis
  - negative sign? 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





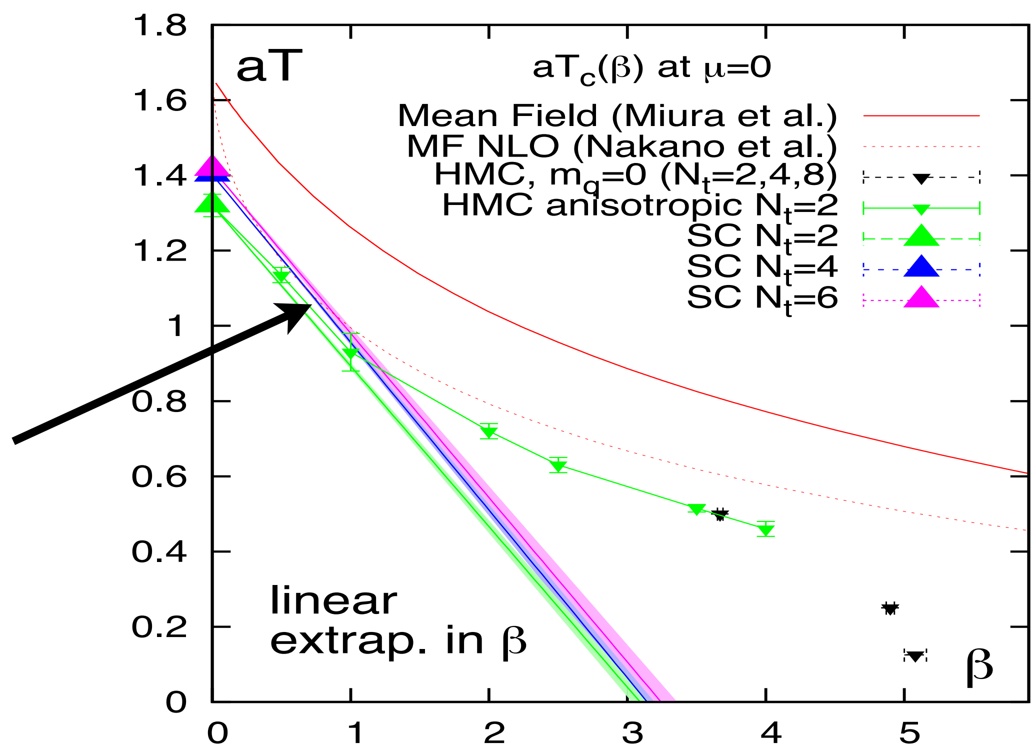


$1/N_t^2$ corrections $\nearrow$

- Chiral transition ($m_q = 0$): 2nd $\rightarrow$ 1rst order as μ increases: *tricritical* point
- finite-N_t corrections $\rightarrow$ 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 → 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*



- $\mu = 0$: crosscheck with HMC ok; linear (aT_c) extrapolation good up to $\beta \sim 1$

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

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

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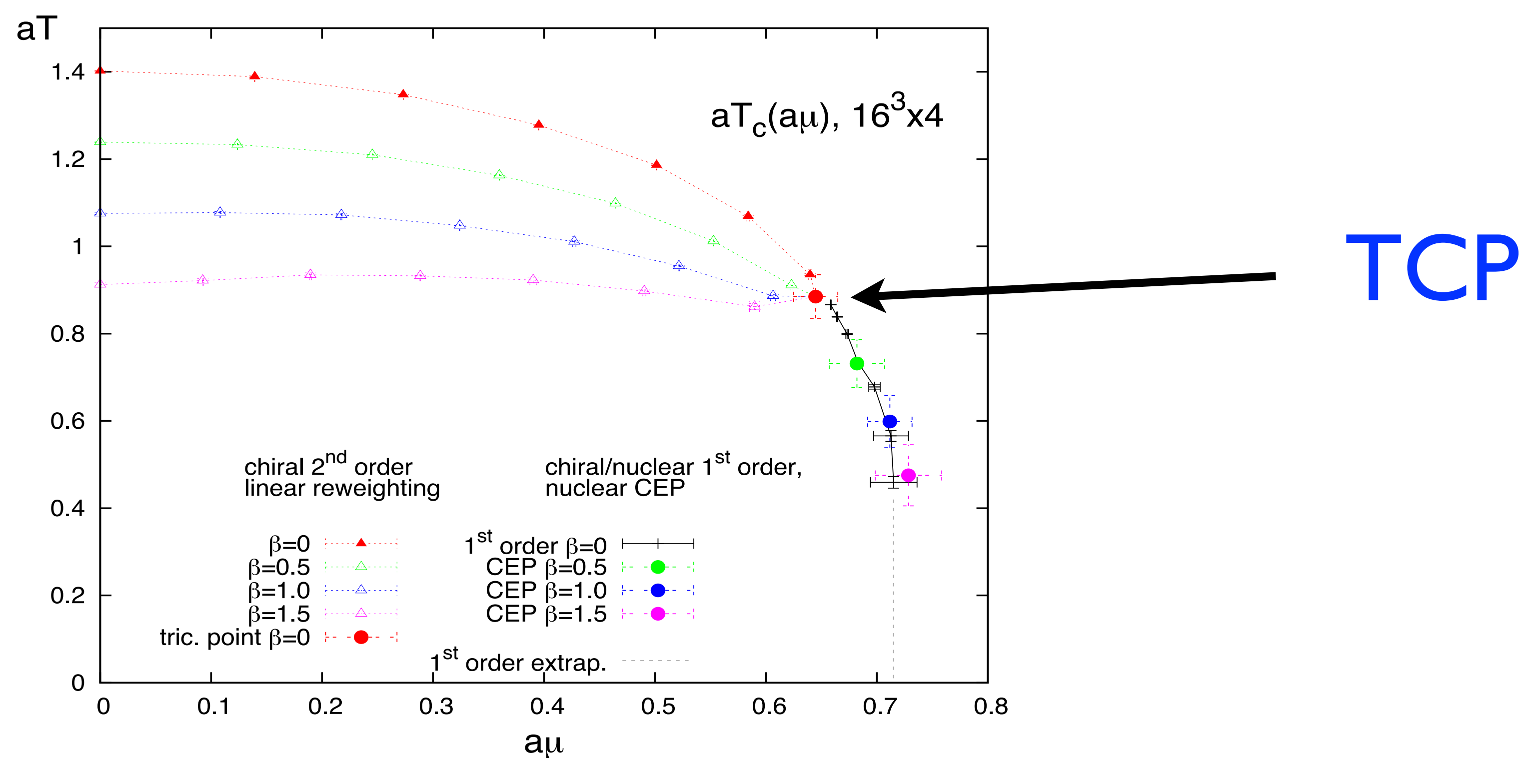

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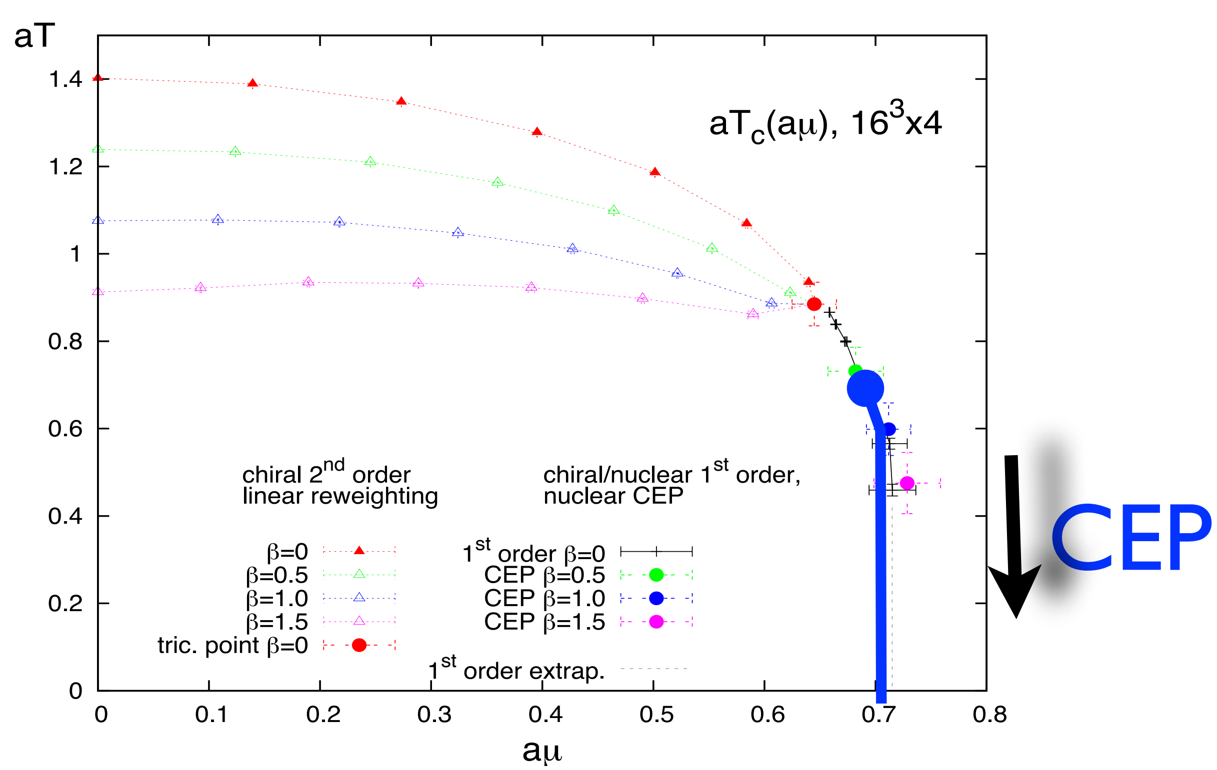
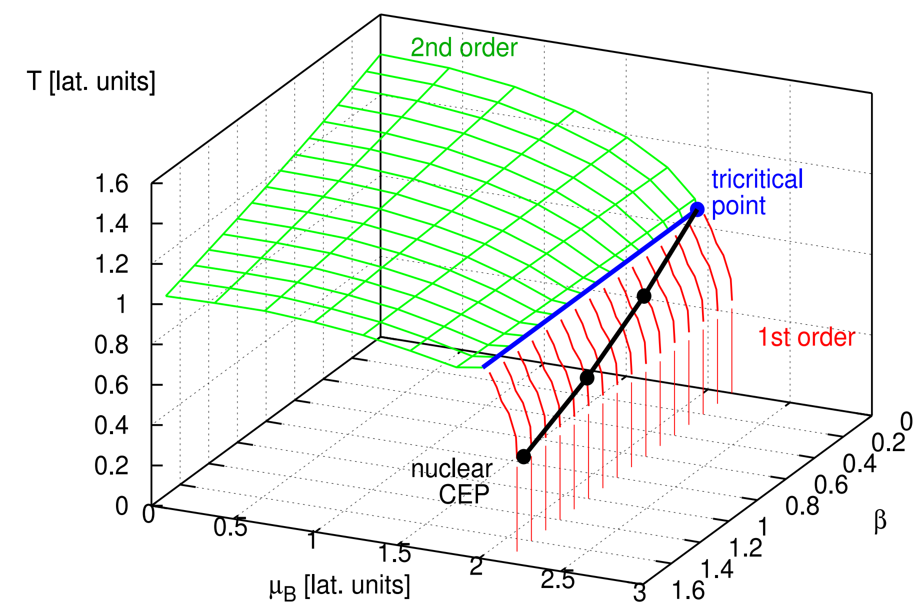




- $\mu = 0$: crosscheck with HMC ok; linear (aT_c) extrapolation good up to $\beta \sim 1$
- $\mu \neq 0$: - phase boundary more "rectangular" with TCP at corner
  - liquid-gas CEP splits and moves down ?

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

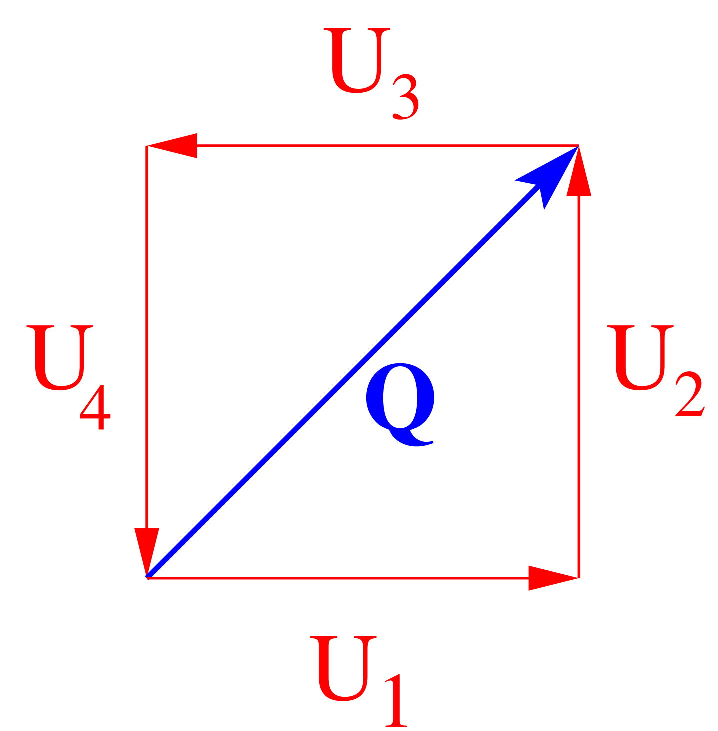
- $\beta \neq 0$: Plaquette 4-link coupling prevents analytic integration of gauge links

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)



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

2-link action → 1-link → 0-link

Vairinhos & PdF, 1409.8442

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

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

Vairinhos & PdF, 1409.8442

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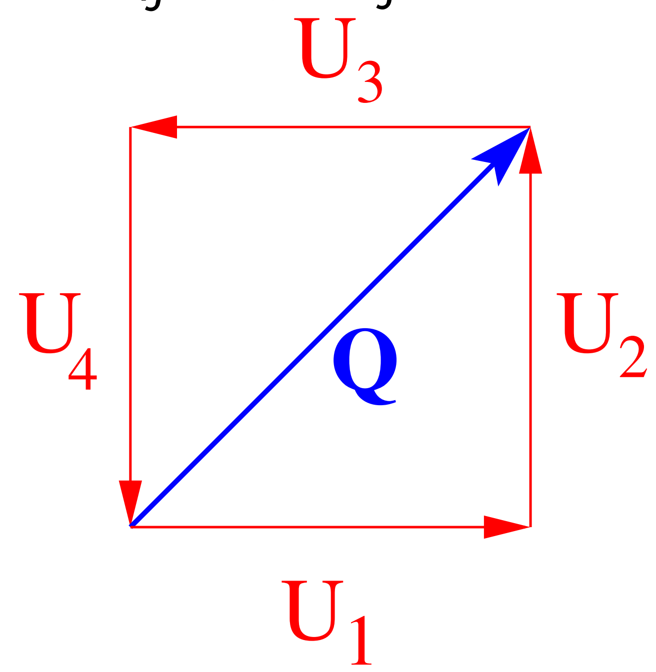
- 4 → 2-link action:

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

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



2-link action → 1-link → 0-link

Vairinhos & PdF, 1409.8442

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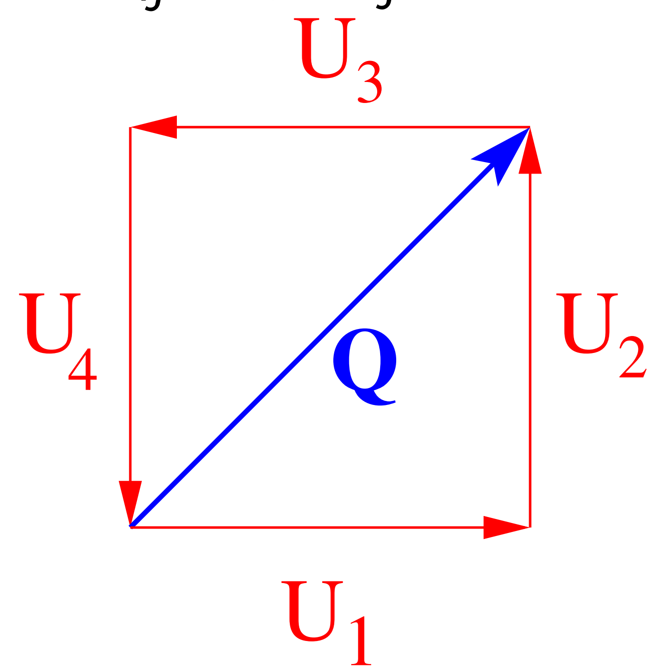
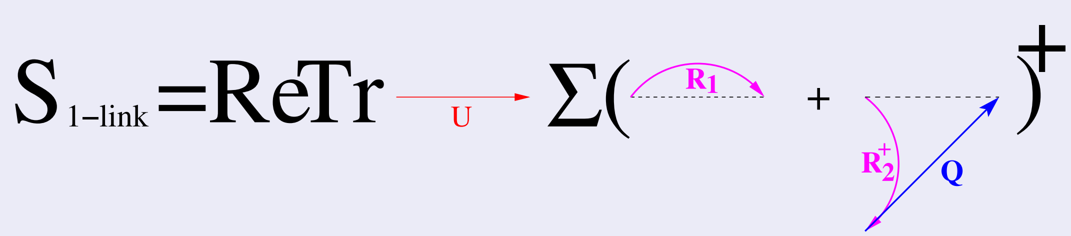
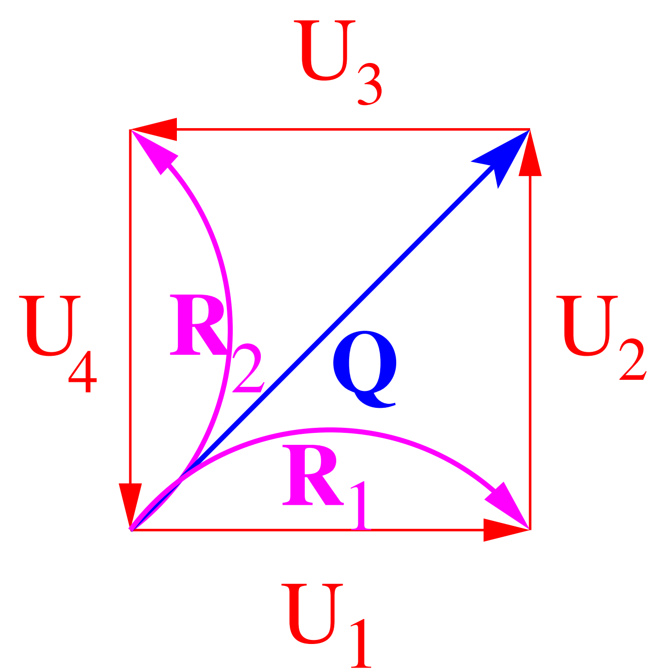


- 2 → 1-link action:

$$Y = (U_1 + QU_2^\dagger),\; X = R_1$$





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

Vairinhos & PdF, 1409.8442

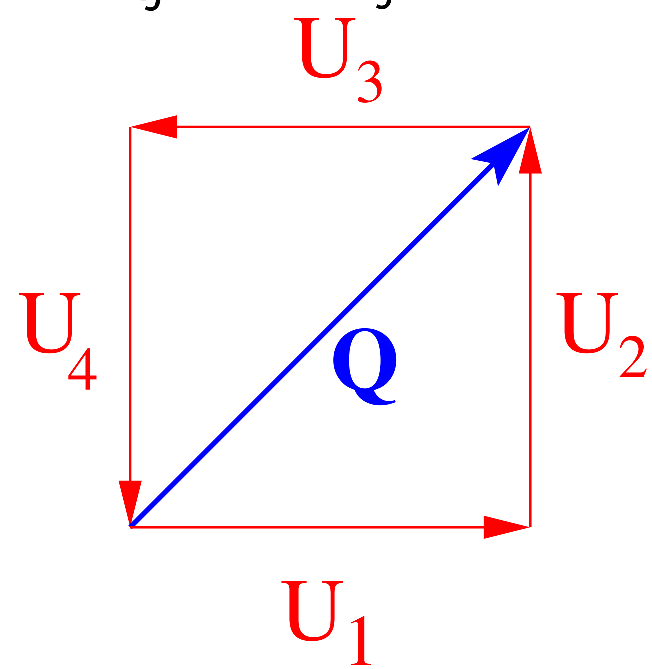
- Hubbard-Stratonovich: $\forall Y \in \mathbf{C}^{N\times N}$, $\quad e^{\mathrm{Tr}Y^\dagger Y} = \mathcal{N}\int dX \; e^{\mathrm{Tr}(X^\dagger Y + XY^\dagger)}$

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

- $4 \to 2$-link action:

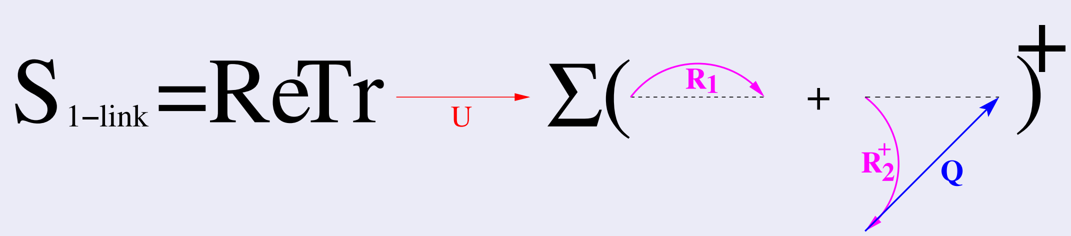
$Y = (U_1 U_2 + U_4^\dagger U_3^\dagger),\ X = Q$

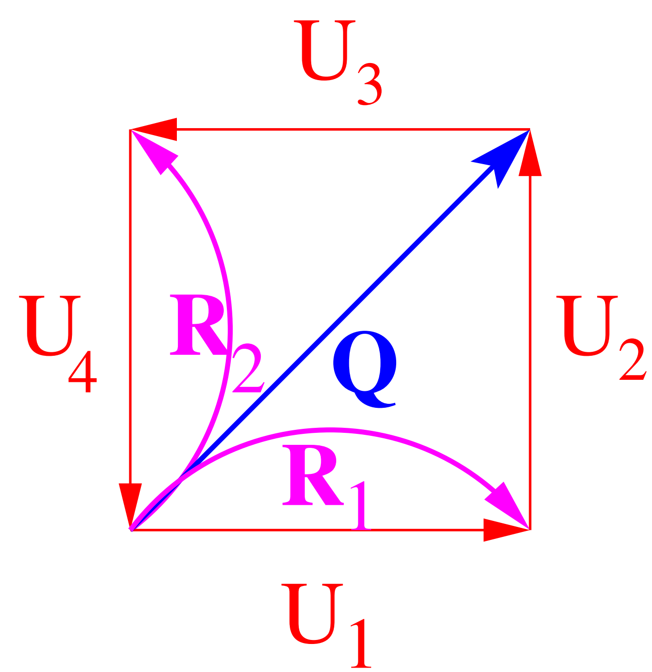
$$S_{2-\mathrm{link}} = \mathrm{ReTr}\ Q^\dagger(U_1 U_2 + U_4^\dagger U_3^\dagger)$$



- $2 \to 1$-link action:

$Y = (U_1 + QU_2^\dagger),\ X = R_1$





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

The road ahead w/Helvio Vairinhos

- Simulate the 1-link and 0-link YM gauge action Done! 1409.8442
- Simulate $U(1)$ gauge + fermions (no chemical potential) at $\beta > 0$
- $U(1) \rightarrow SU(3)$
- $\mu \neq 0$

Caveat: when $\beta > 0$, the complex auxiliary fields Q & R re-introduce a sign pb

In physical terms: color neutrality is only true for distances $\gtrsim 1/\Lambda_{\rm QCD}$

$\rightarrow$ how large can we take β before the sign pb becomes unmanageable?

Cautious optimism...

Backup

Complex Langevin 80's revival Seiler, Stamatescu, Aarts, Sexty,..

- Real action S: Langevin evolution in Monte-Carlo time τ Parisi-Wu

$\frac{\partial\phi}{\partial\tau} = -\frac{\delta S[\phi]}{\delta\phi} + \eta$, ie. drift force + noise

Can prove: $\langle W[\phi]\rangle_\tau = \frac{1}{Z}\int \mathcal{D}\phi \exp(-S[\phi]) W[\phi]$

- Complex action S ? Parisi, Klauder, Karsch, Ambjorn,..

Drift force complex $\rightarrow$ complexify field $(\phi^R + i\phi^I)$ and simulate as before

With luck: $\langle W[\phi^R + i\phi^I]\rangle_\tau = \frac{1}{Z}\int \mathcal{D}\phi \exp(-S[\phi]) W[\phi]$

- Only change since 1980's: adaptive stepsize $\rightarrow$ runaway sols disappear

- Gaussian example:

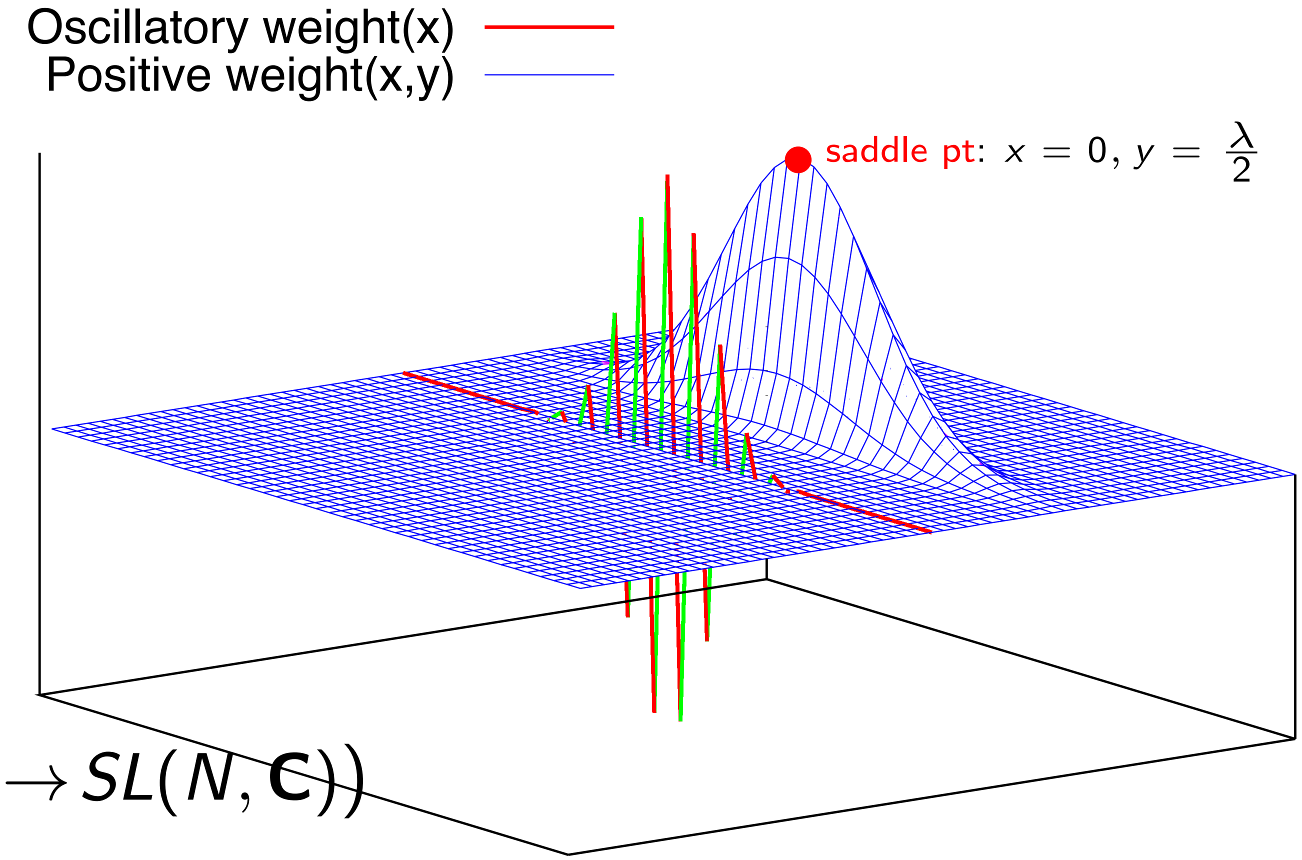
$Z(\lambda) = \int dx \exp(-x^2 + \mathbf{i}\lambda\mathbf{x})$

Complexify:

$\frac{d}{d\tau}(x + iy) = -2(x + iy) + i\lambda + \eta$

For any observable W,

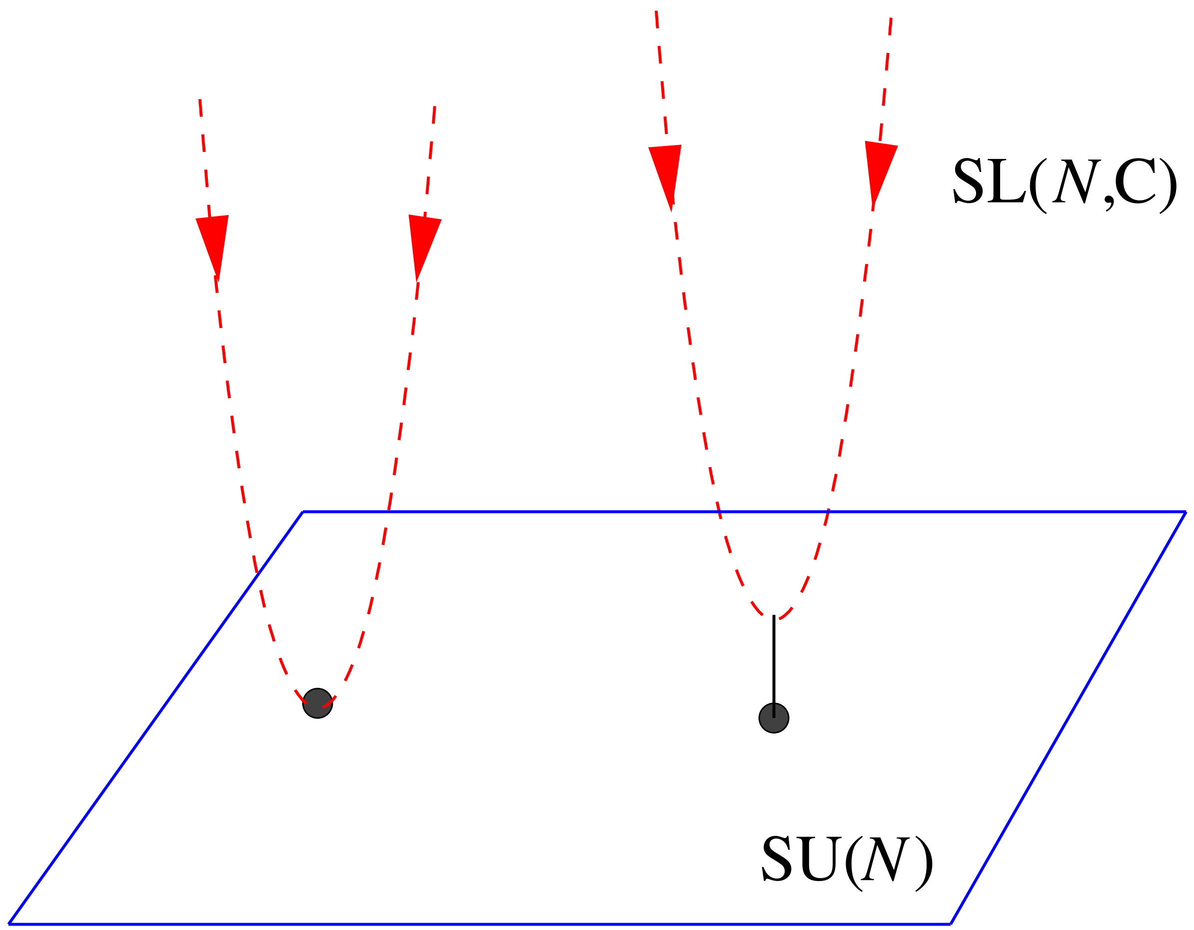
$\langle W(x + iy)\rangle_\tau = \langle W(x)\rangle_Z$

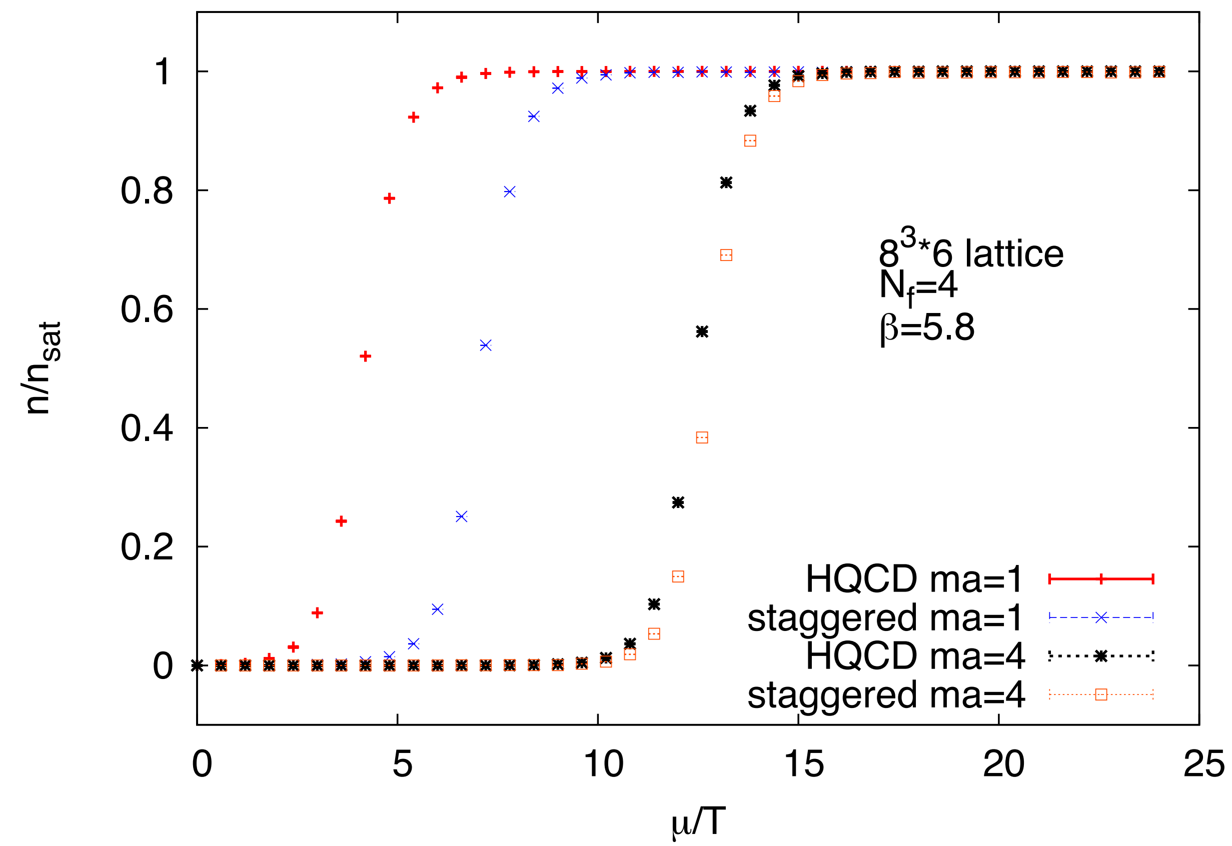


- Flat directions going to ∞? $(SU(N) \rightarrow SL(N, \mathbf{C}))$
- $S = \mathrm{Tr}\log \rightarrow$ cut??

Complex Langevin II

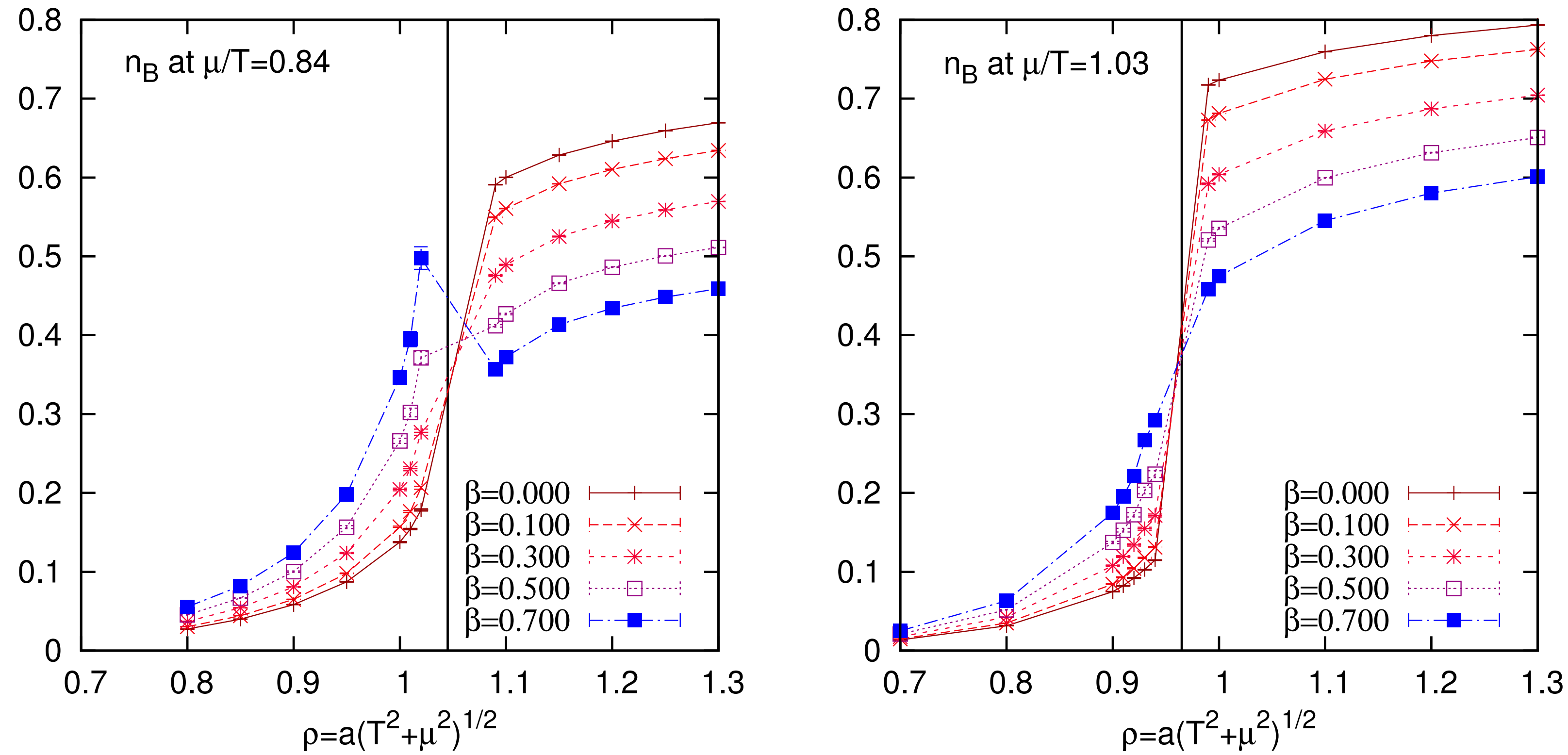
Seiler, Stamatescu, Aarts, Sexty,..





- Control excursions in imaginary direction by *gauge-cooling* in $SL(N, \mathbf{C})$
  Should make no difference except for roundoff error
- Large values of μ/T explored with heavy quarks:
  results OK checked against static quarks
- First results for light quarks at high T (chirally symmetric phase)
  Are they correct?
- NB: complex Langevin gives wrong results in disordered phase of 3d XY model
  Aarts & James: 1005.3468

Liquid-gas endpoint moves to lower temperatures as β increases



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