Progress toward the phase diagram of QCD from the lattice

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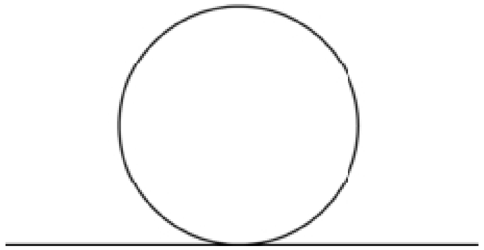
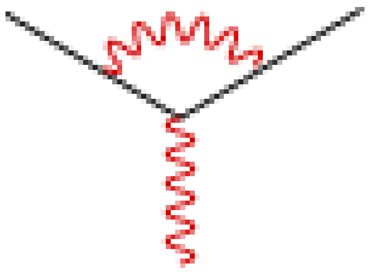


ϕ^4: mass diverges with cutoff ?



QED: e diverges with cutoff ?

changes with gauge ?

$\Longrightarrow$ Renormalization

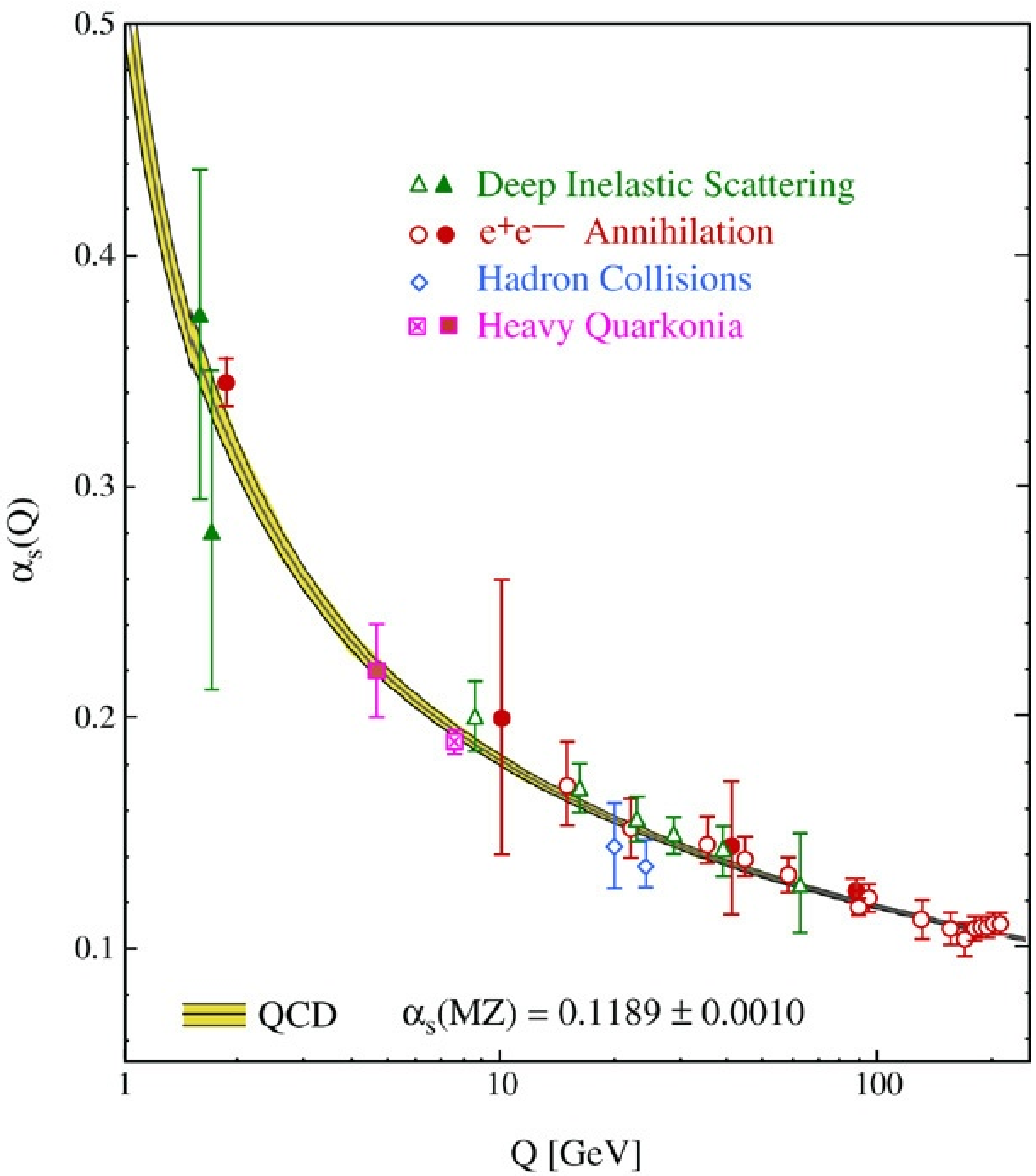
The lattice is the only known gauge-invariant, non-perturbative regulator of QFT

1974: invented by Ken Wilson 

1980: first Yang-Mills simulation by Mike Creutz 

Basic properties of QCD

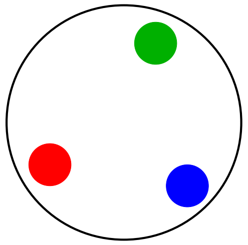
- QCD describes properties of *quarks* (cf. electrons – fermions) interacting by exchanging *gluons* (cf. photons – bosons)
- QCD is *asymptotically free*: weaker interaction at higher energy



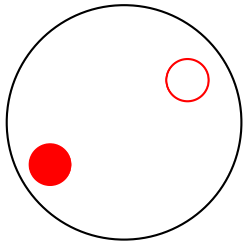
The flip side of asymptotic freedom: “infrared slavery”

- Strong coupling at low energy $\rightarrow$ non-perturbative
- Quarks are confined into color-neutral (color singlet) bound-states (hadrons):

qqq baryons: proton & neutron (ordinary matter), ...



$q\bar{q}$ mesons: pion (lightest), kaon, rho, ...

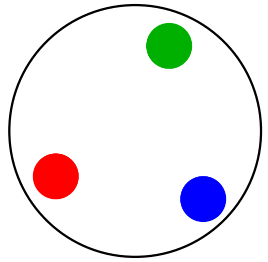


Exotics: glueballs, tetraquarks $qq\bar{q}\bar{q}$, pentaquarks $qqqq\bar{q}$, etc...

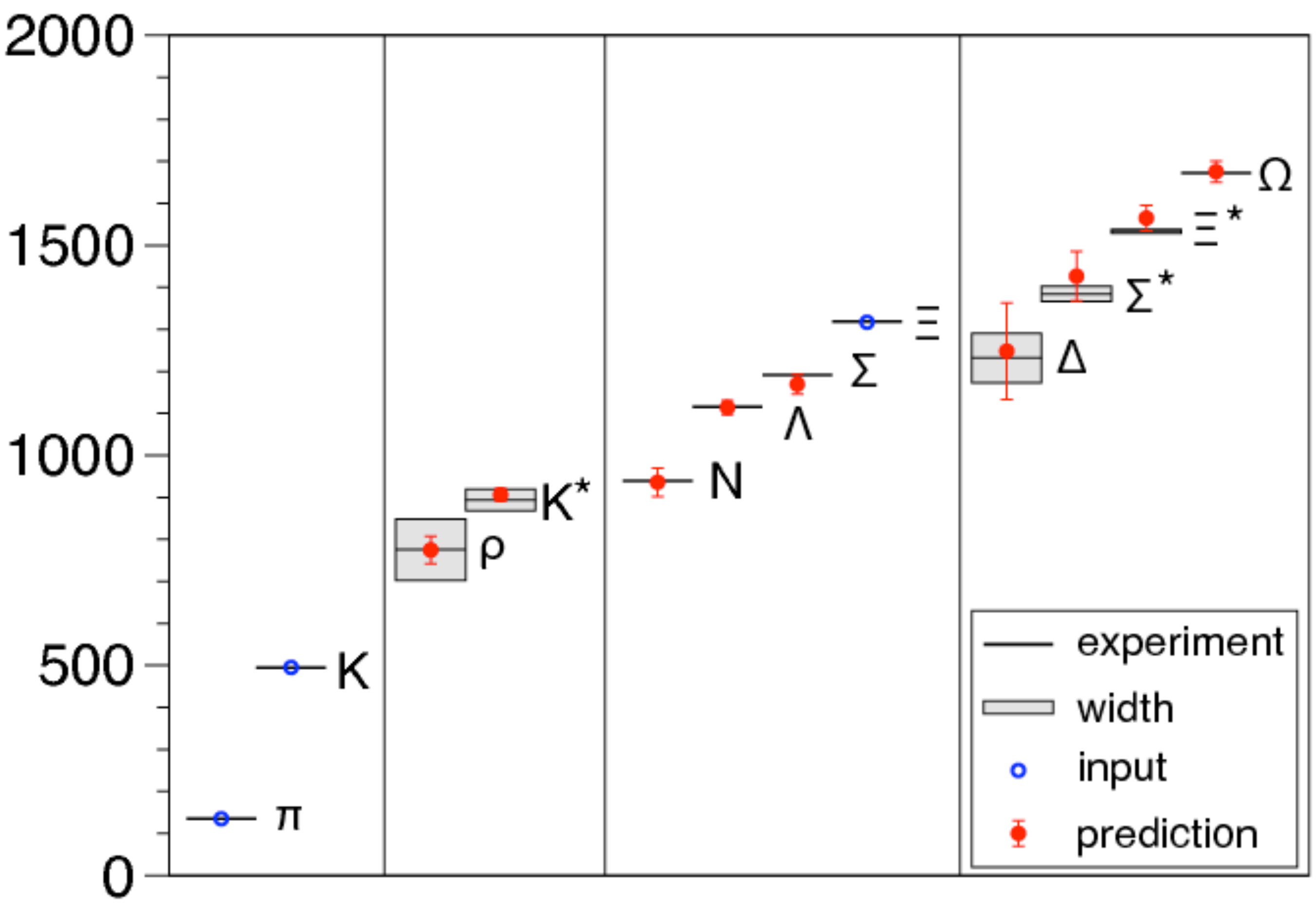
In principle, all calculable by Lattice QCD simulations

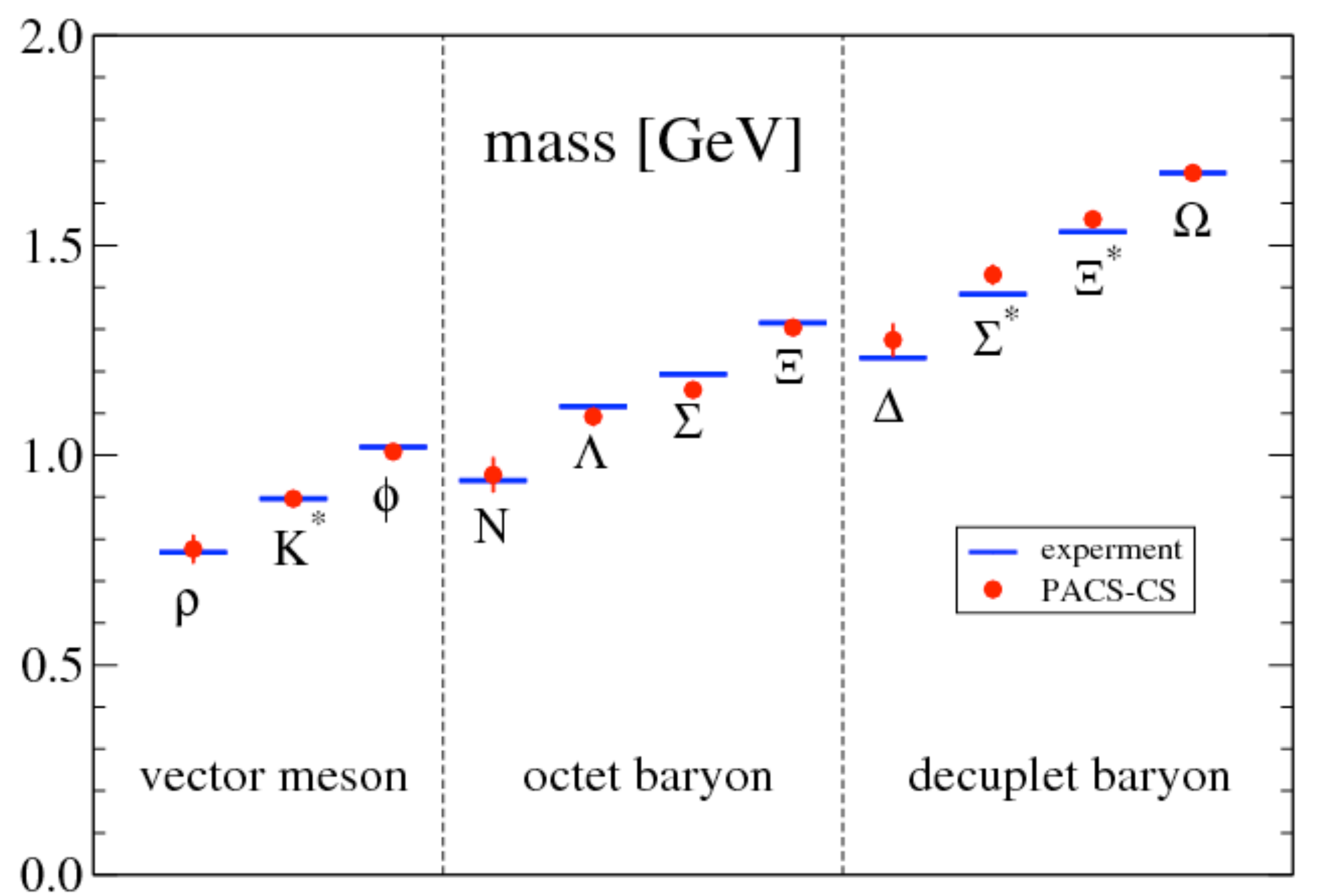
Scope of lattice QCD simulations: Physics of color singlets

* "One-body" physics: confinement
  hadron masses
  form factors, etc..



Example: hadron masses





BMW collaboration

arXiv:0906.3599 $\longrightarrow$ Science

PACS-CS collaboration

arXiv:0807.1661

Follow-up: neutron-proton mass diff.

arXiv:1406.4088 $\longrightarrow$ Science

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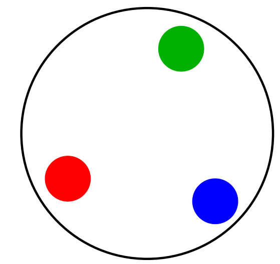
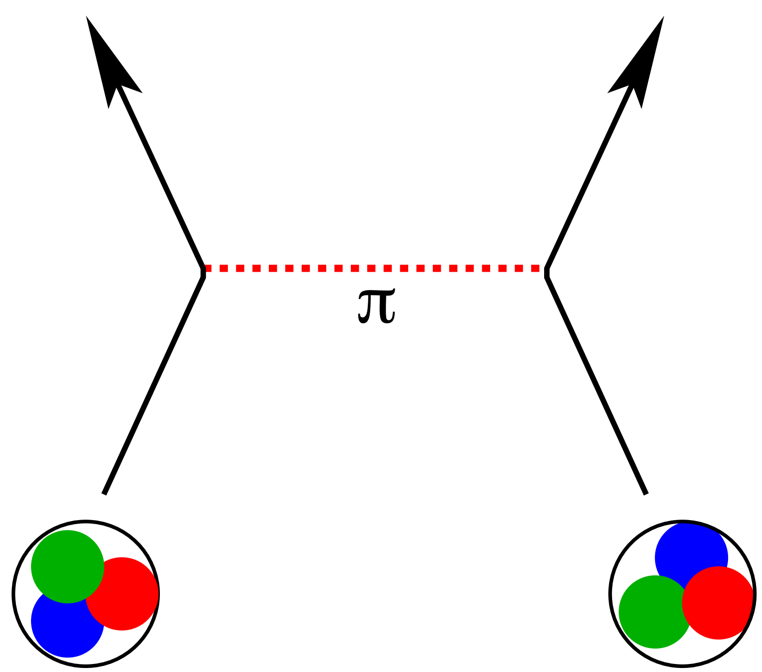


** “Two-body” physics: nuclear interactions
pioneers Hatsuda et al, Savage et al



hard-core
+
pion exchange?

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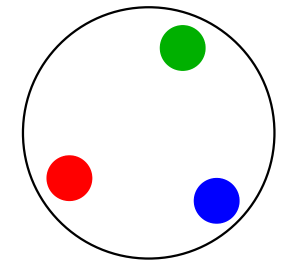

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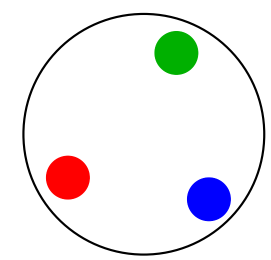

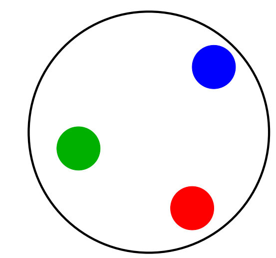

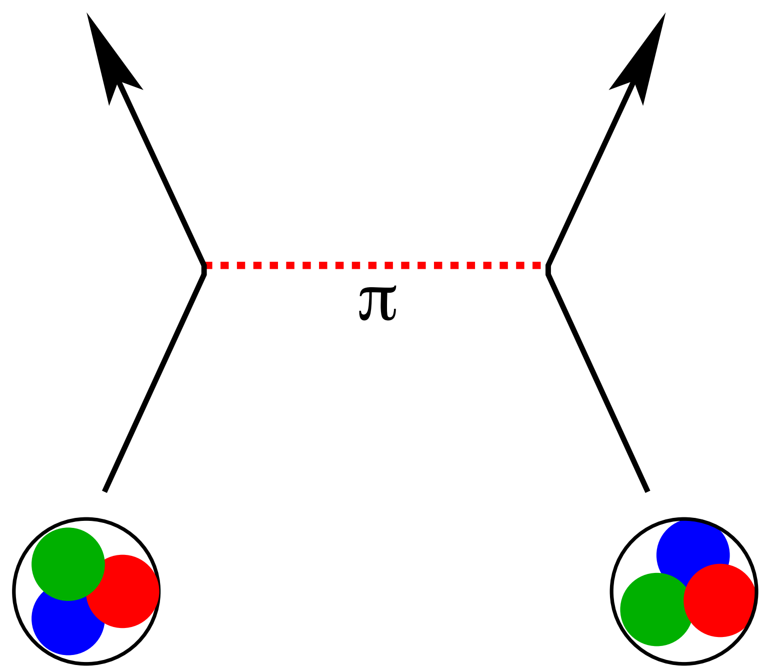

hard-core
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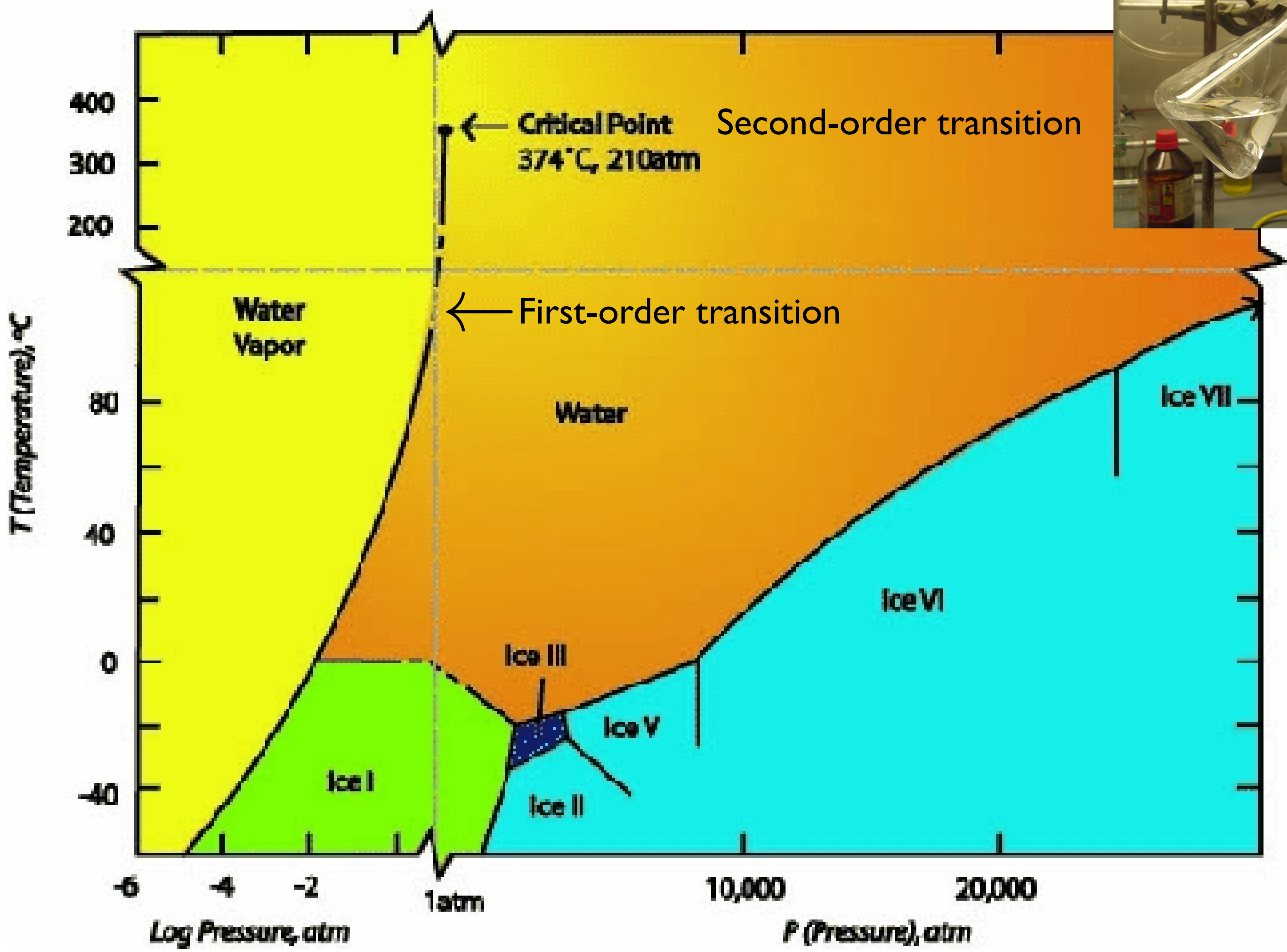
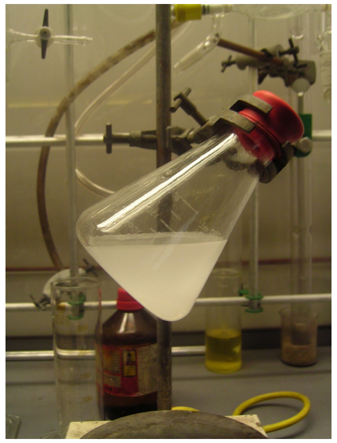
*** Many-[composite]-body physics: nuclear matter
phase diagram vs (temperature T, density $\leftrightarrow$ μ_B)

Motivation

What happens to matter when it is heated and/or compressed?

Water changes its state when heated or compressed

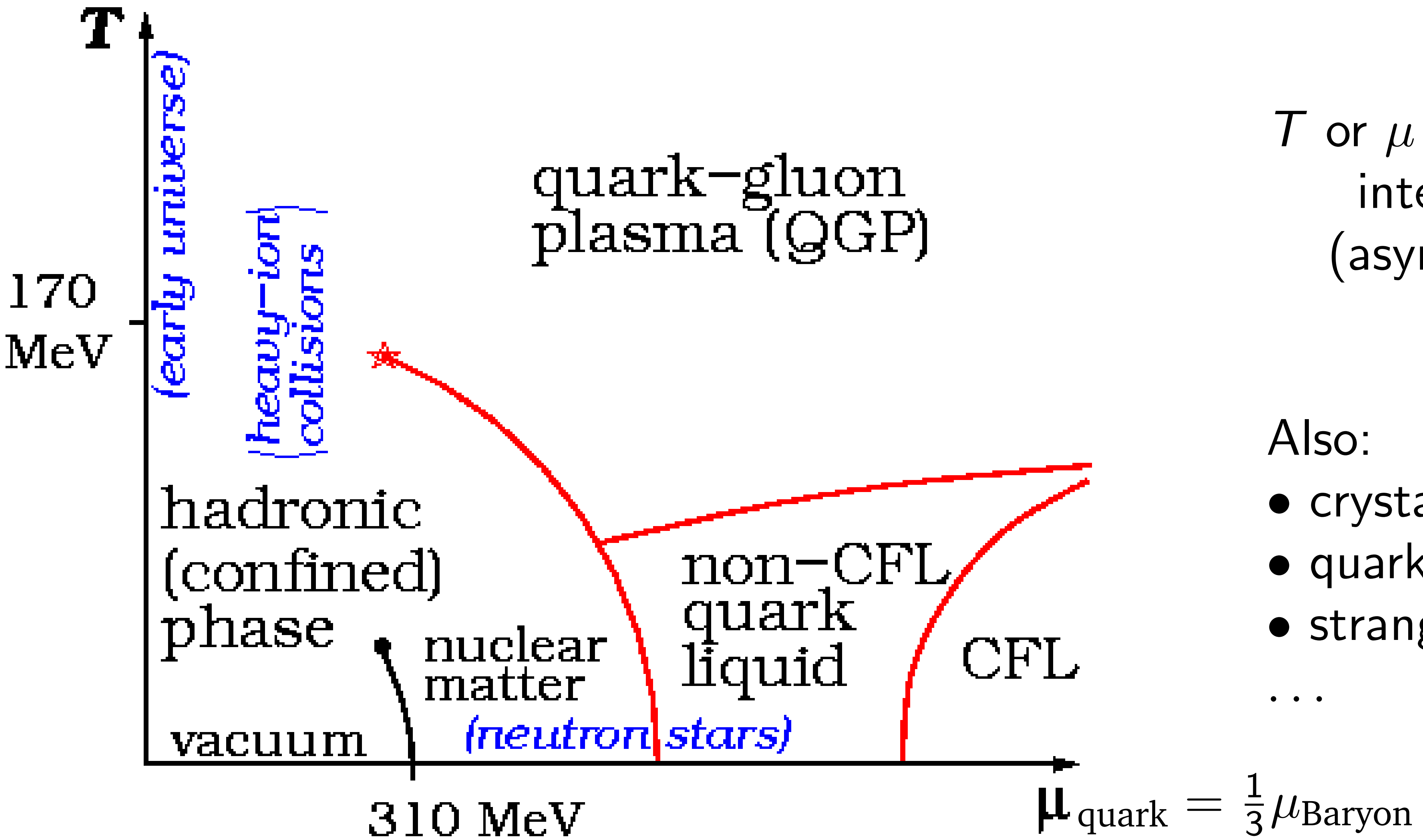




critical opalescence

What happens to quarks and gluons when heated or compressed?

The wonderland phase diagram of QCD from Wikipedia



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

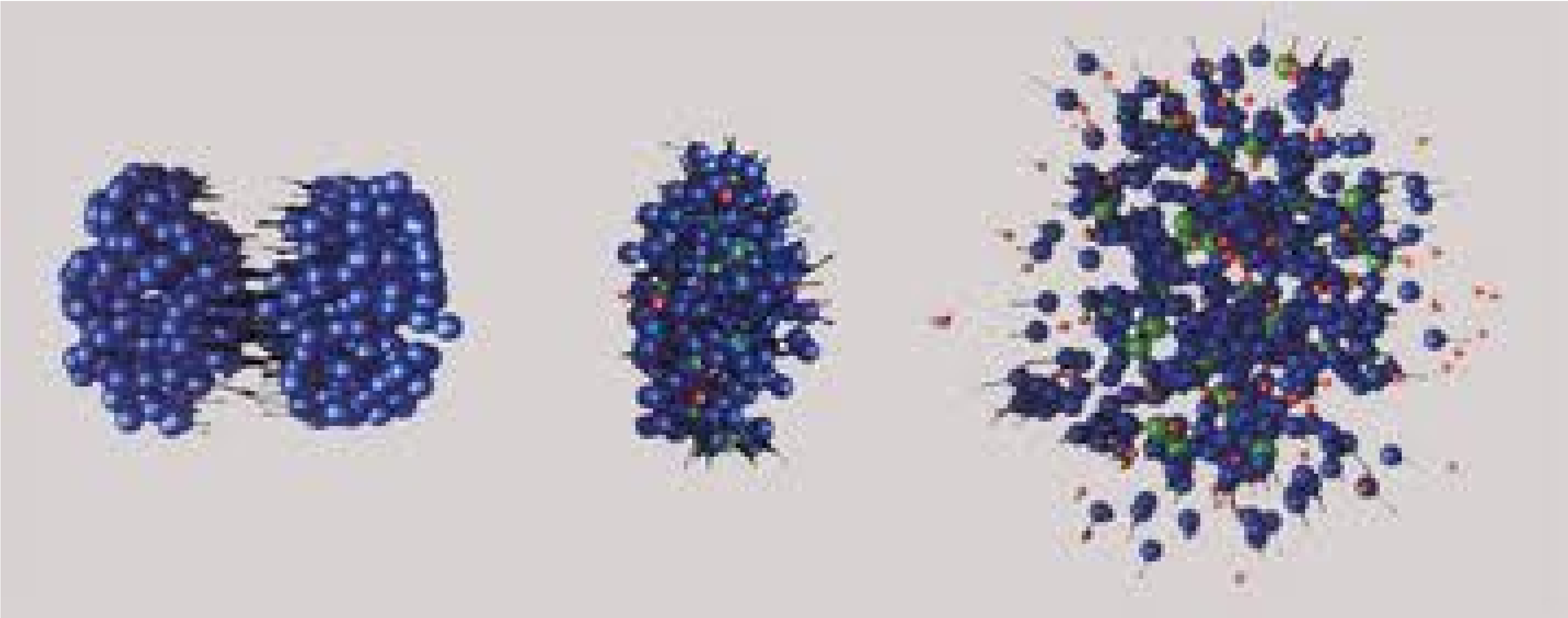
Also:

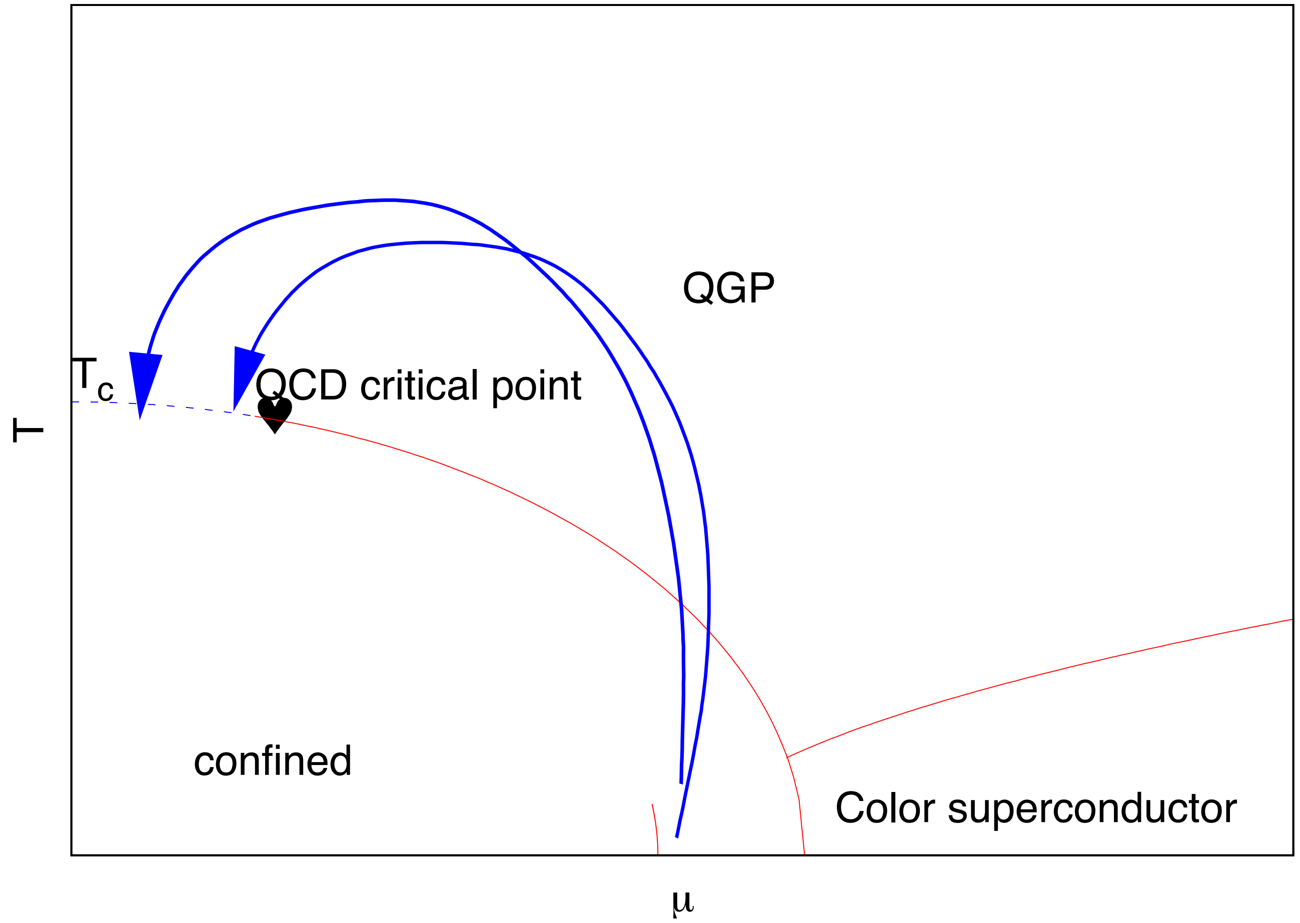
- crystal phase(s)
- quarkyonic phase
- strangelets

...

Caveat: everything in red is a conjecture

Heavy-ion collisions





Knobs to turn:

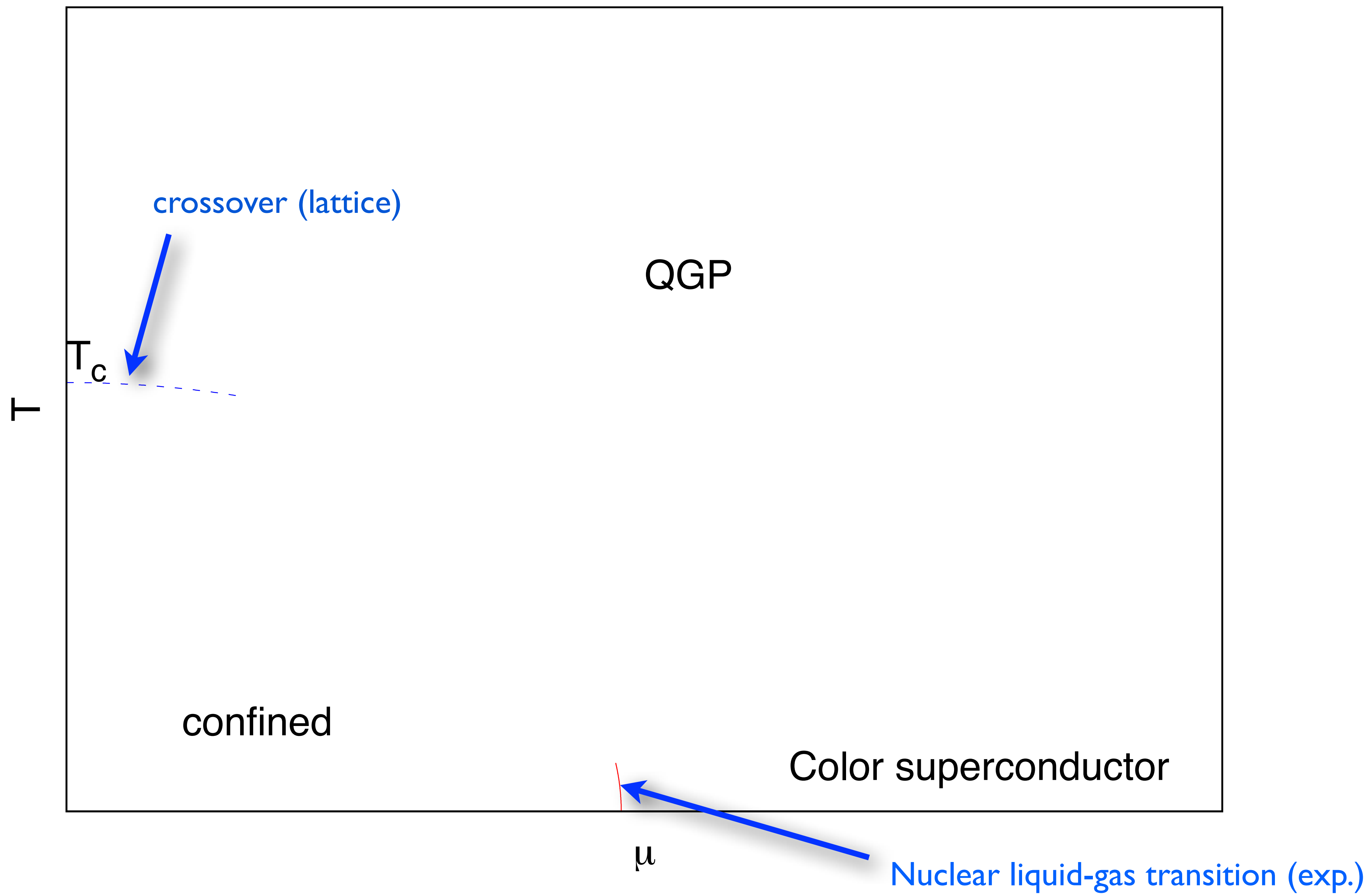
- atomic number of ions
- collision energy $\sqrt{s}$

So far, no sign of QCD critical point (esp. RHIC beam energy scan)

"critical opalescence" ?

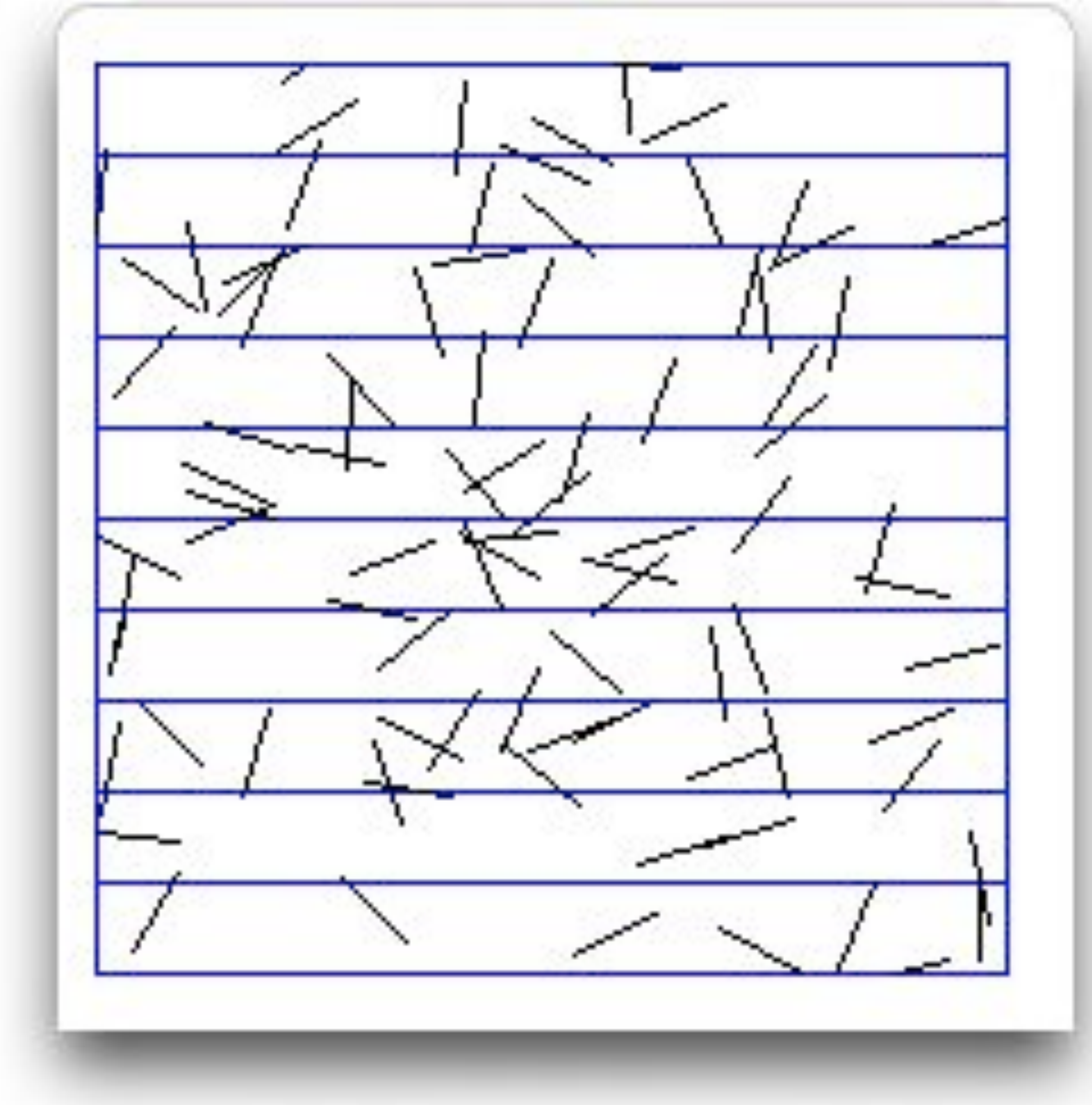
Finite μ: what is known?

Minimal, possible phase diagram



Monte Carlo? sign problem *as soon as* $\mu \neq 0$

The first Monte Carlo experiment (1777)



Probability of intersection: $\frac{2}{\pi}$

The extraordinary efficiency of Monte Carlo

Typical: $Z = \sum_{\text{states}} \exp[-S(\text{state})]$; $\langle W \rangle = \frac{1}{Z} \sum_{\text{states}} W(\text{state}) \exp[-S(\text{state})]$

Number of states $\sim$ exp(volume V)

Monte Carlo: approximate Z by random subset of n states

Law of large numbers $\rightarrow$ error $\sim n^{-1/2}\ \forall V$

How to sample $Z = \sum_{\text{states}} \exp[-S(\text{state})]$?

- Random sampling: Pick states with *uniform* prob., give them weight $\exp(-S)$
- Importance sampling: Pick states with prob. $\exp(-S)$, give them *uniform* weight

Metropolis et al, 1953

Monte Carlo: no pain, no gain...

Monte Carlo highly efficient: *importance sampling* $\mathrm{Prob(conf)} \propto \exp[-S(\mathrm{conf})]$

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

$$\exists \text{ conf s.t. "Boltzmann weight" } \exp[-S(\mathrm{conf})] \notin \mathbb{R}_{\geq 0}$$

No probabilistic interpretation — Monte Carlo impossible??

- Examples:

- real-time quantum evolution:

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

- Hubbard model:

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

  complex except at half-filling (additional symmetry)

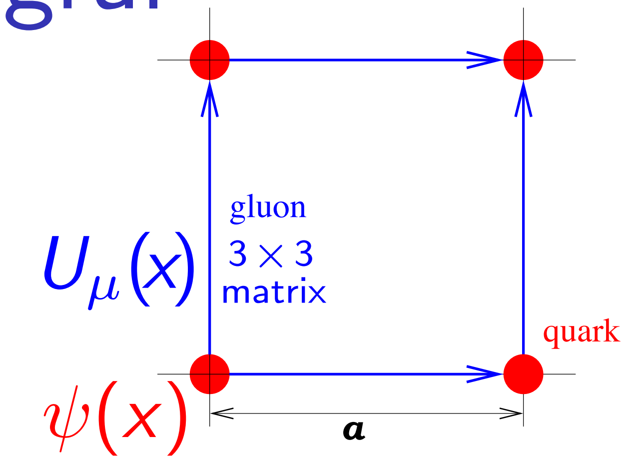
- QCD at non-zero density / chemical potential:

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

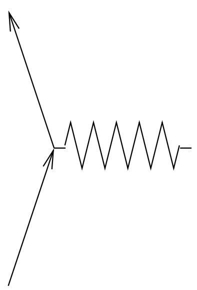
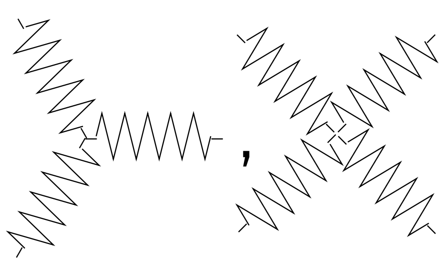
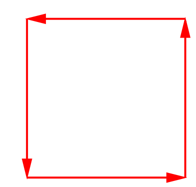
  complex unless $\mu = 0$ or pure imaginary (additional symmetry)

Lattice QCD: Euclidean path integral

space + imag. time $\to$ $4d$ 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 $\bar\psi \not{D} \psi$
  -  $\longrightarrow$ $\beta\, \mathrm{Re}\mathrm{Tr}\, U_P$, U_P plaquette matrix  Yang-Mills action $\frac{1}{4} F_{\mu\nu} F_{\mu\nu}$

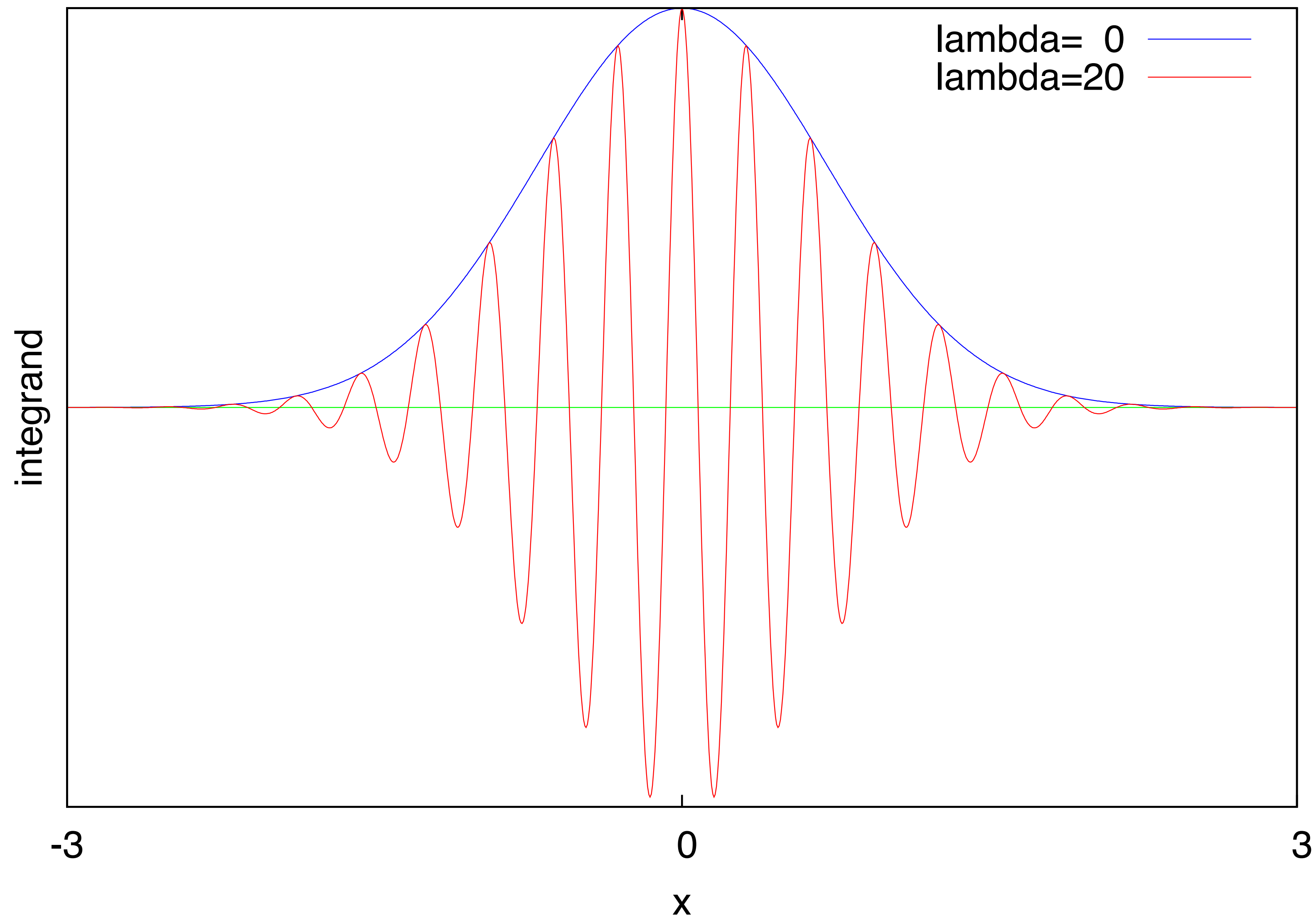
$$a \to 0 \Leftrightarrow \beta = \frac{6}{g_0^2} \to \infty$$

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

$$\mathrm{Prob}(\mathrm{config}\{U\}) \propto \det{}^2 \not{D}(\{U\})\, e^{+\beta \sum_P \mathrm{Re}\mathrm{Tr}\, U_P}$$ 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*" :

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

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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 $\propto \exp(+2\frac{V}{T}\Delta f)$

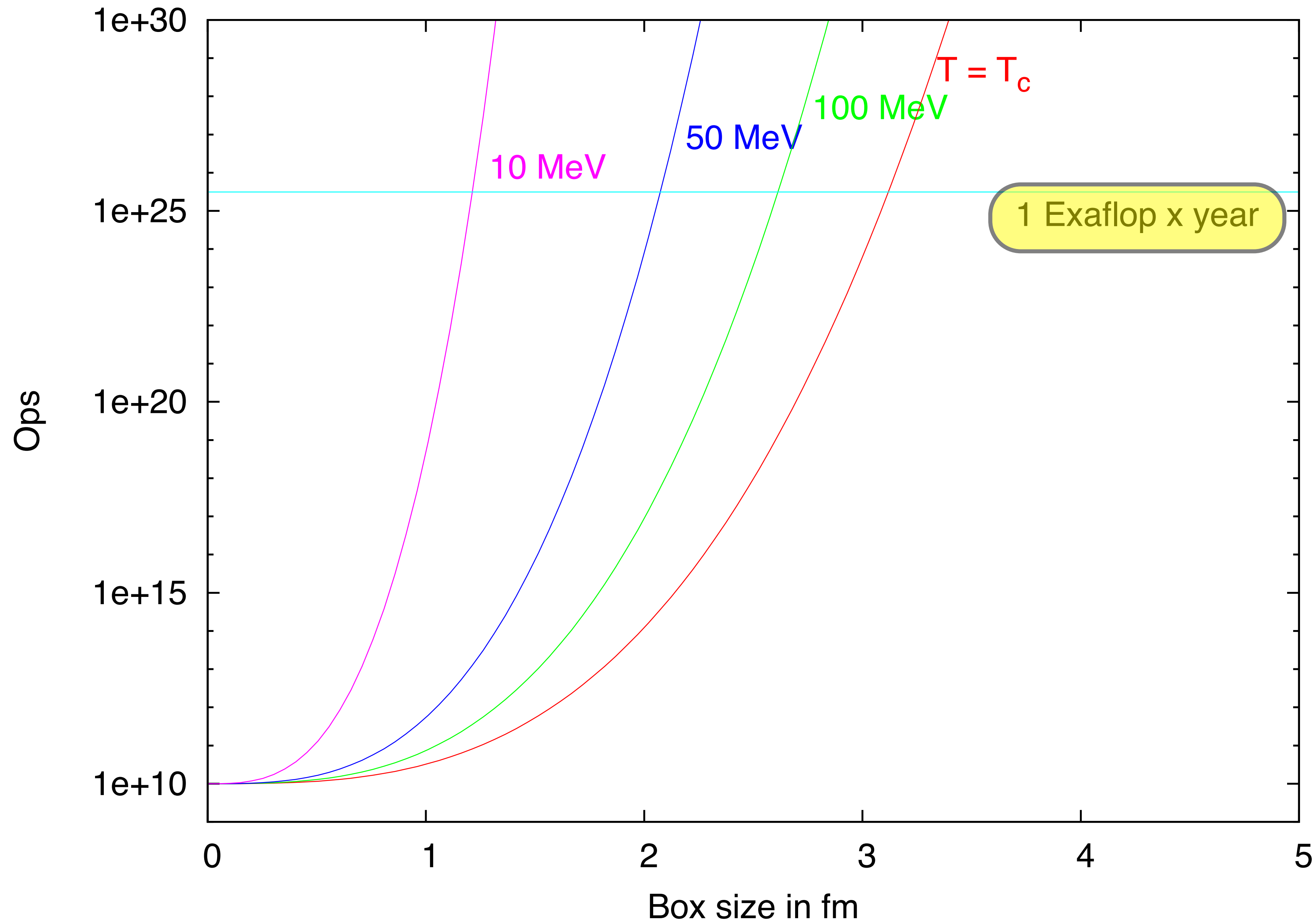
  Large V, low T inaccessible: signal/noise ratio degrades exponentially

"Figure of merit" Δf: measures severity of sign pb.

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

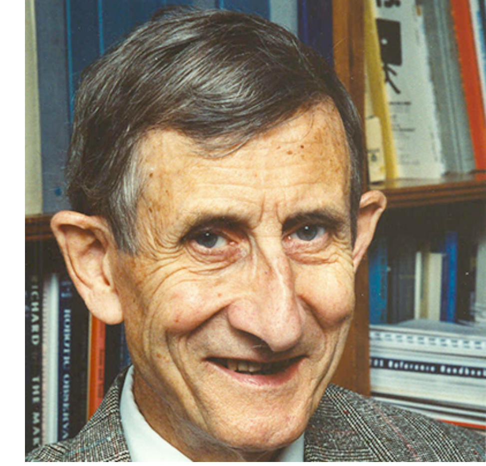
CPU effort to study matter at nuclear density in a box of given size

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 $\propto \exp(2\frac{V}{T}\underbrace{\rho_{\text{nucl.}}(m_B - 3/2m_\pi)}_{\Delta f})$

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

Taylor expansion, imaginary μ, strong coupling expansion,...

- Birds: *solve* the sign pb
  - solve QCD ?
  - find "QCD-ersatz" which can be made sign-pb free

Complex Langevin, Lefschetz thimble – fermion bags, QC_2D, isospin μ,...

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

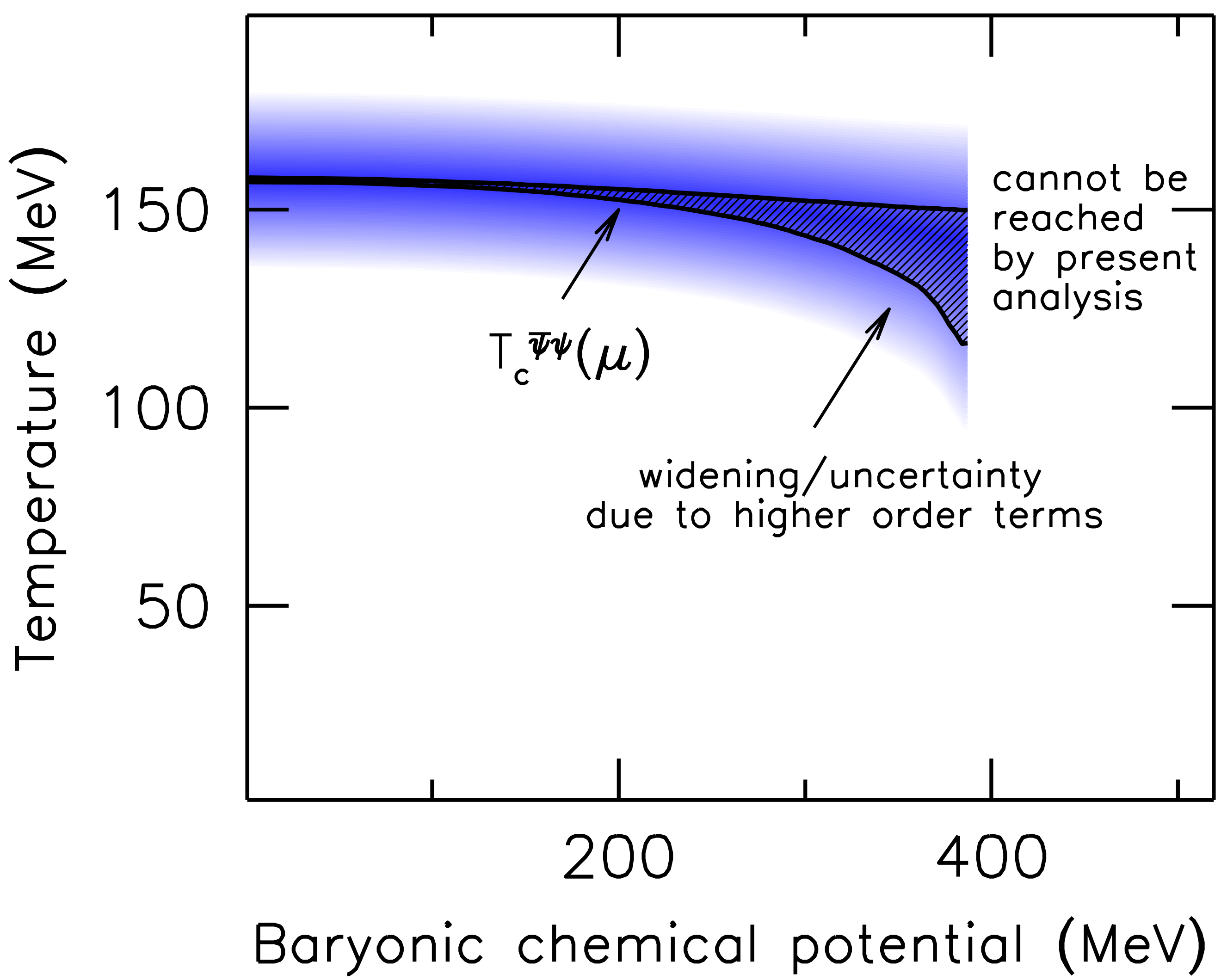
First frog steps: $\frac{\mu}{T} \lesssim 1$

Approximate $\langle W \rangle (\frac{\mu}{T})$ by truncated Taylor expansion: $\sum_{k=0}^{\mathbf{n}} c_k(T) \left(\frac{\mu}{T}\right)^k$

- Measure $c_k, k = 0, .., n$ in a sign-pb-free $\mu = 0$ simulation
- Cheaper variant: fit $c_k, k = 0, .., n$ to results of *imaginary* μ simulations

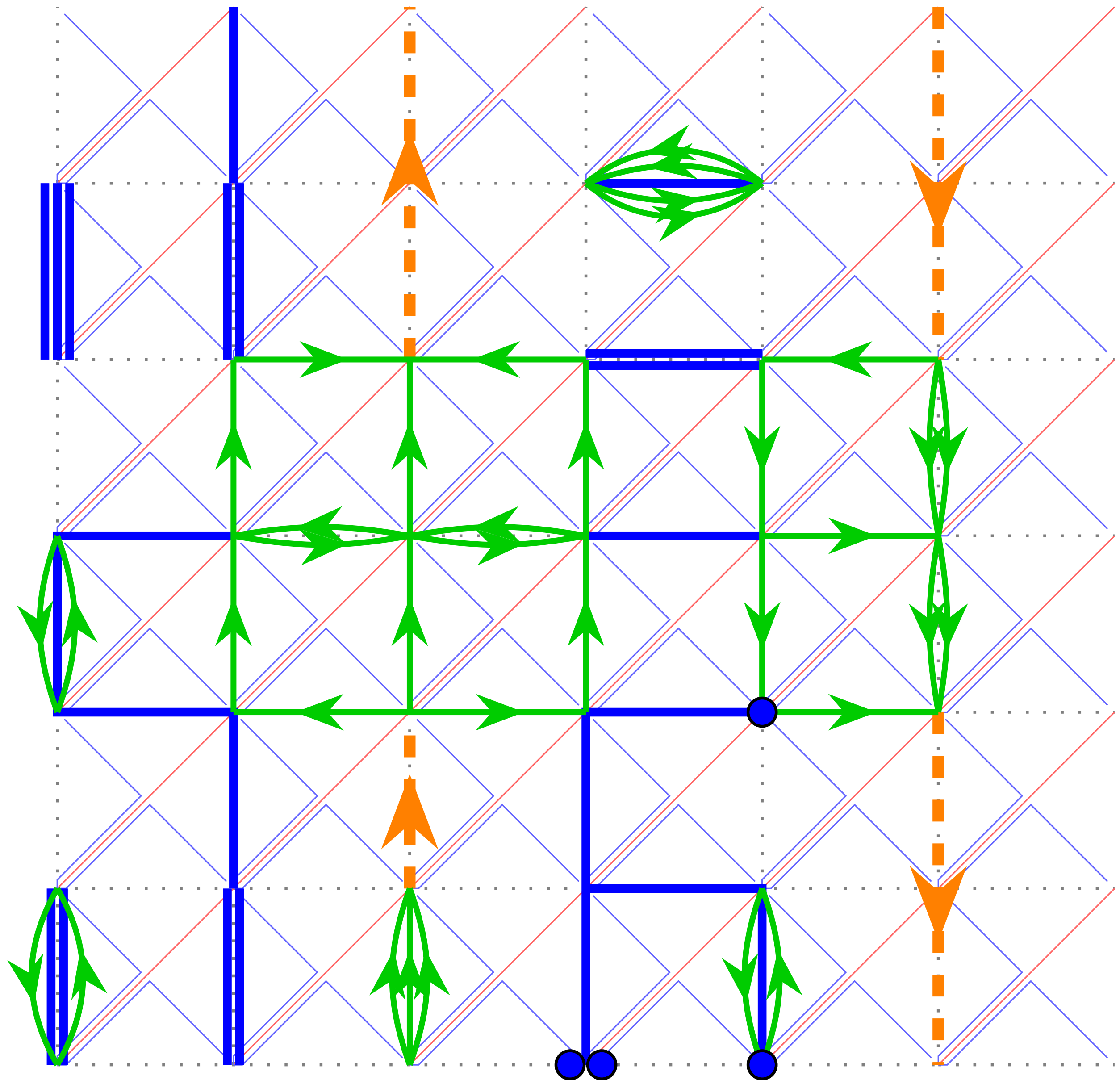
State of the art: Fodor et al, 1507.07510

Crossover temp. versus chem. pot.



Crafty frog: “diagrammatic” Monte Carlo

QCD with graphs: why and how?



Exploit feature of QCD: *fermions* (quarks) & *bosons* (gluons), integrated sequentially

Motivation: how to make the sign problem milder?

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

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

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

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

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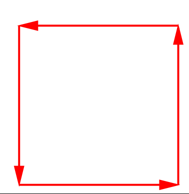
Usual:
- integrate over quarks analytically $\rightarrow \det(\{U\})$
- Monte Carlo over gluon fields $\{U\}$

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

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

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

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

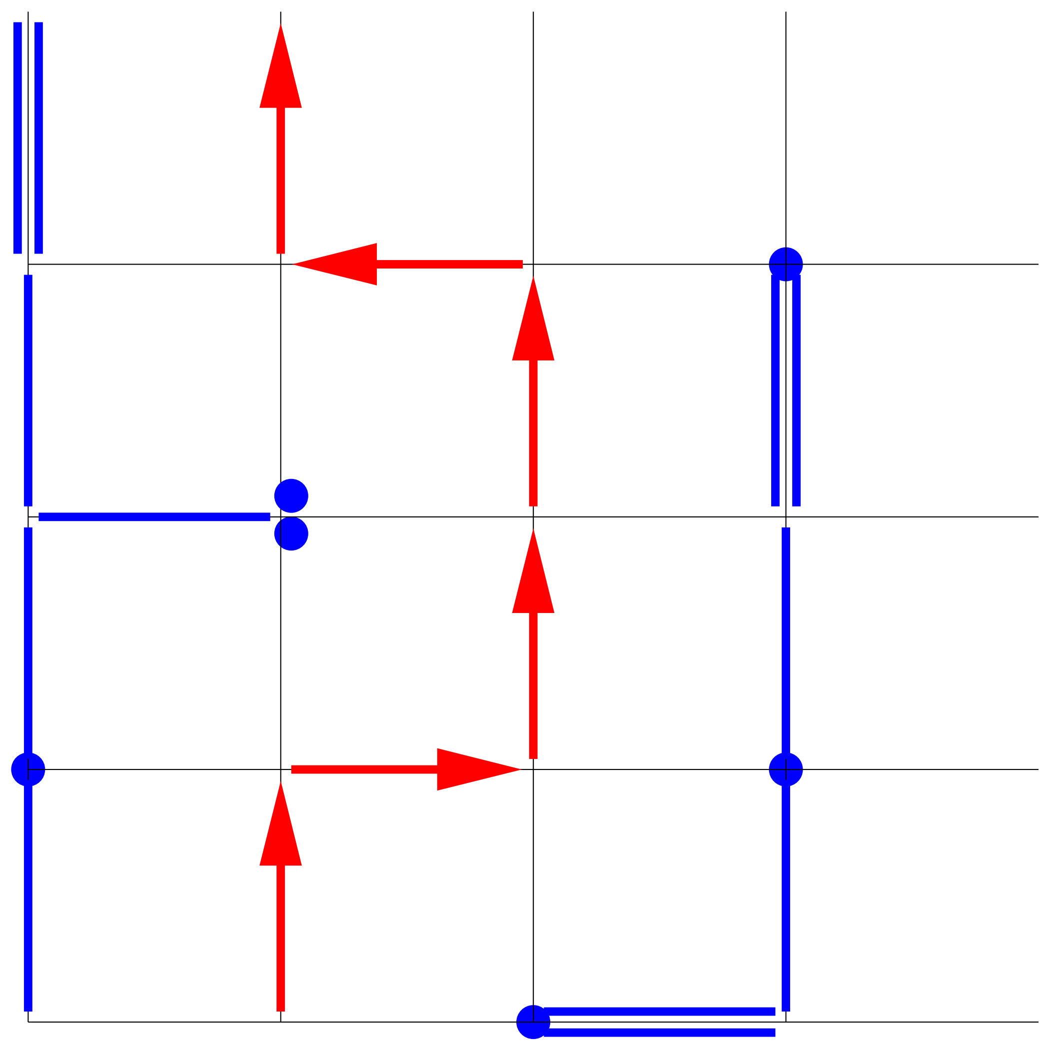
Product of 1-link integrals performed analytically

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



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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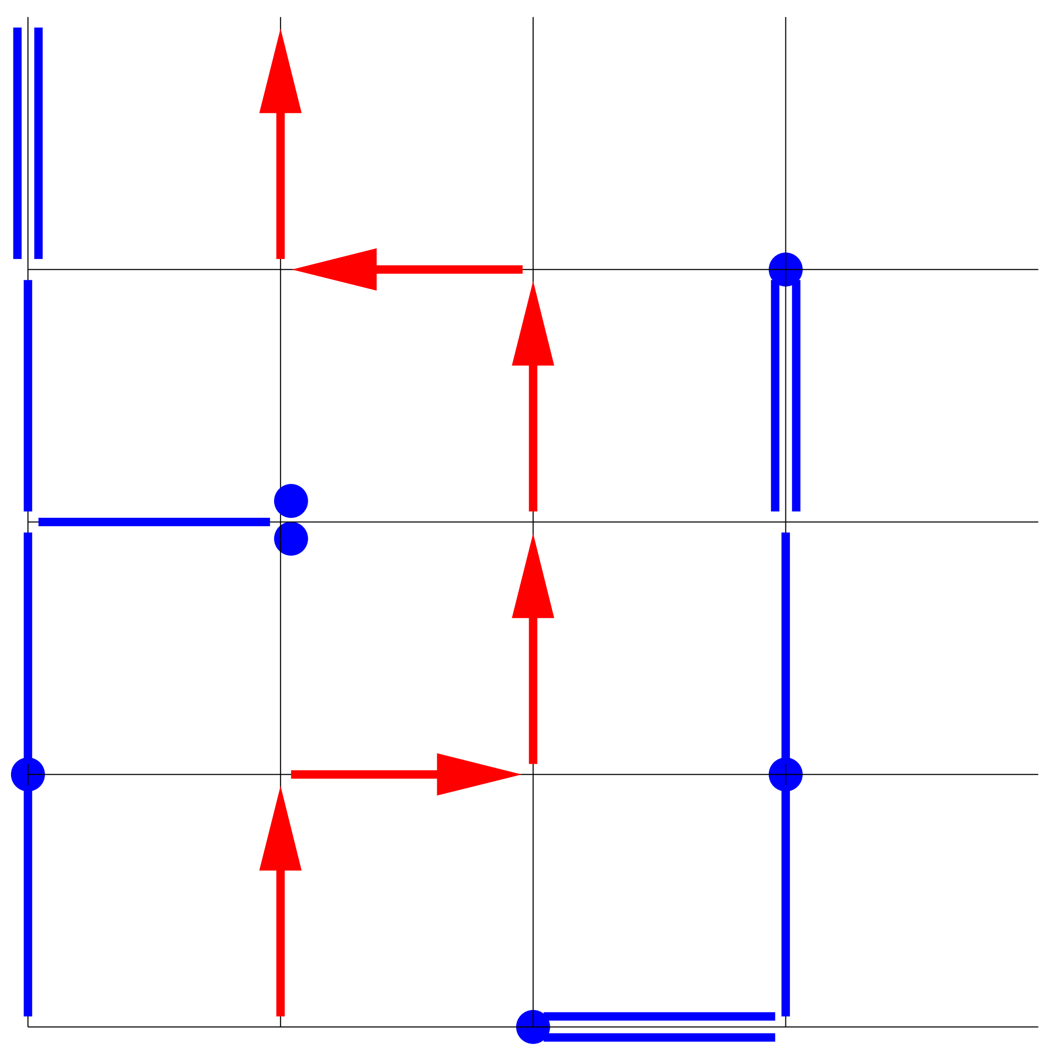

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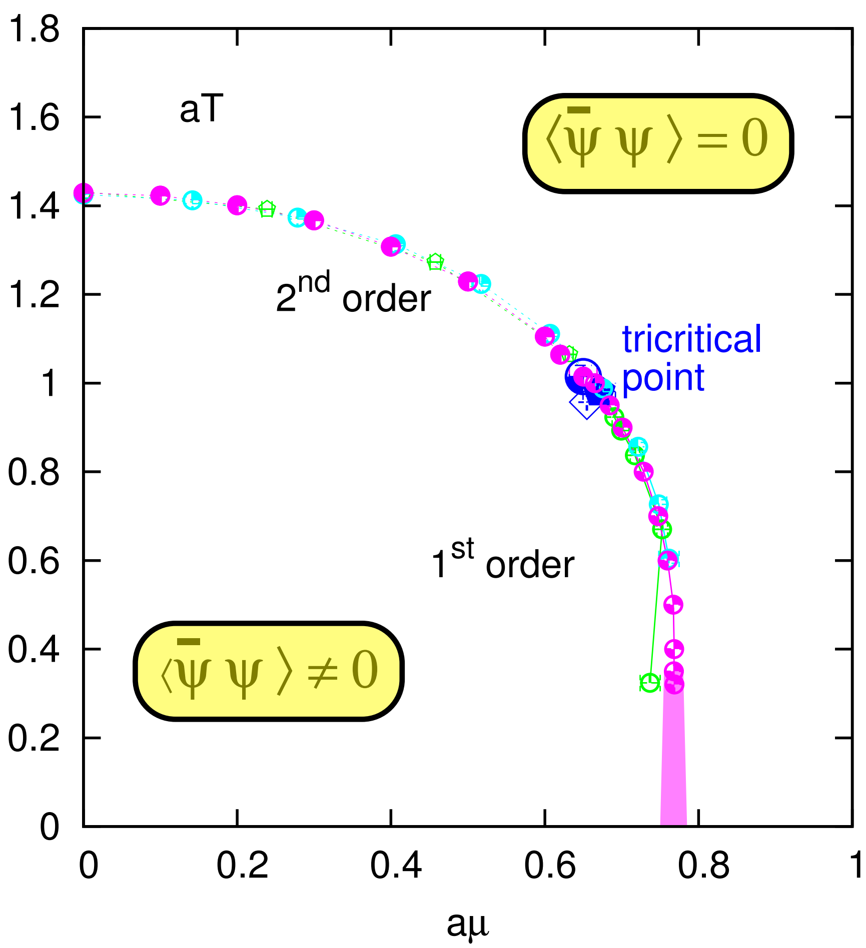
The dense (crystalline) phase:
1 baryon per site; no space left
$\rightarrow \quad \langle \bar{\psi}\psi \rangle = 0$

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

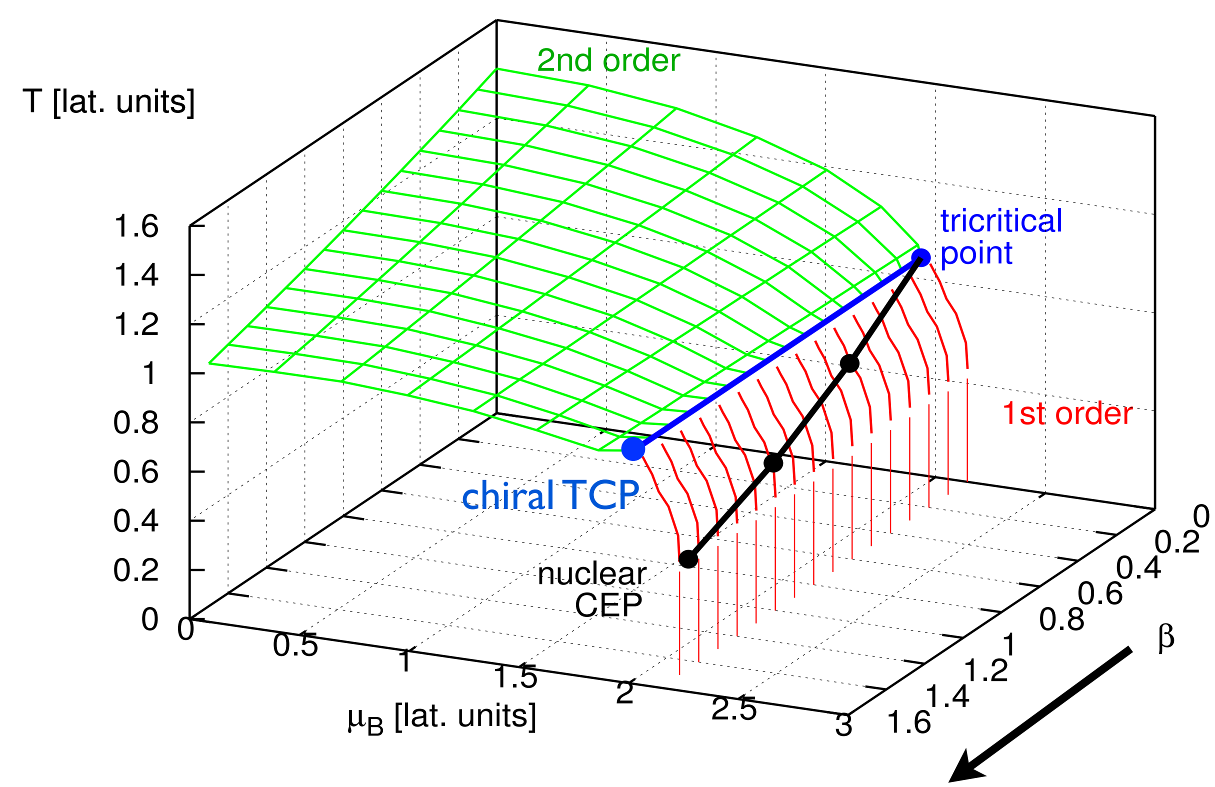
Results $\beta \approx 0$ w/Unger, Langelage, Philipsen

- Sign pb almost gone: accessible volumes multiplied by 10^4
- Phase diagram ($m_q = 0$): chiral phase transition

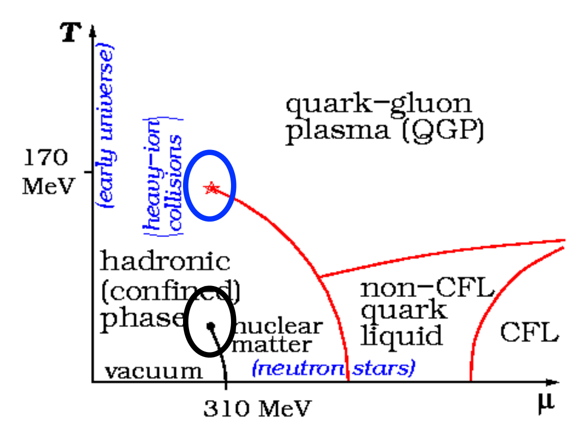
$\beta = 0$



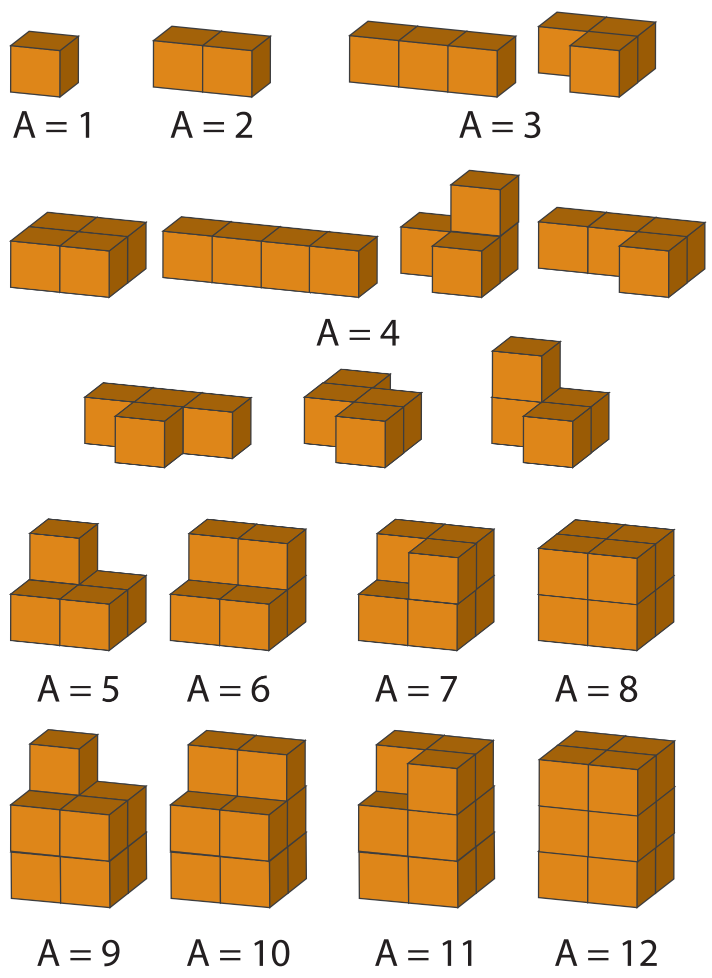
$\mathcal{O}(\beta)$ corrections

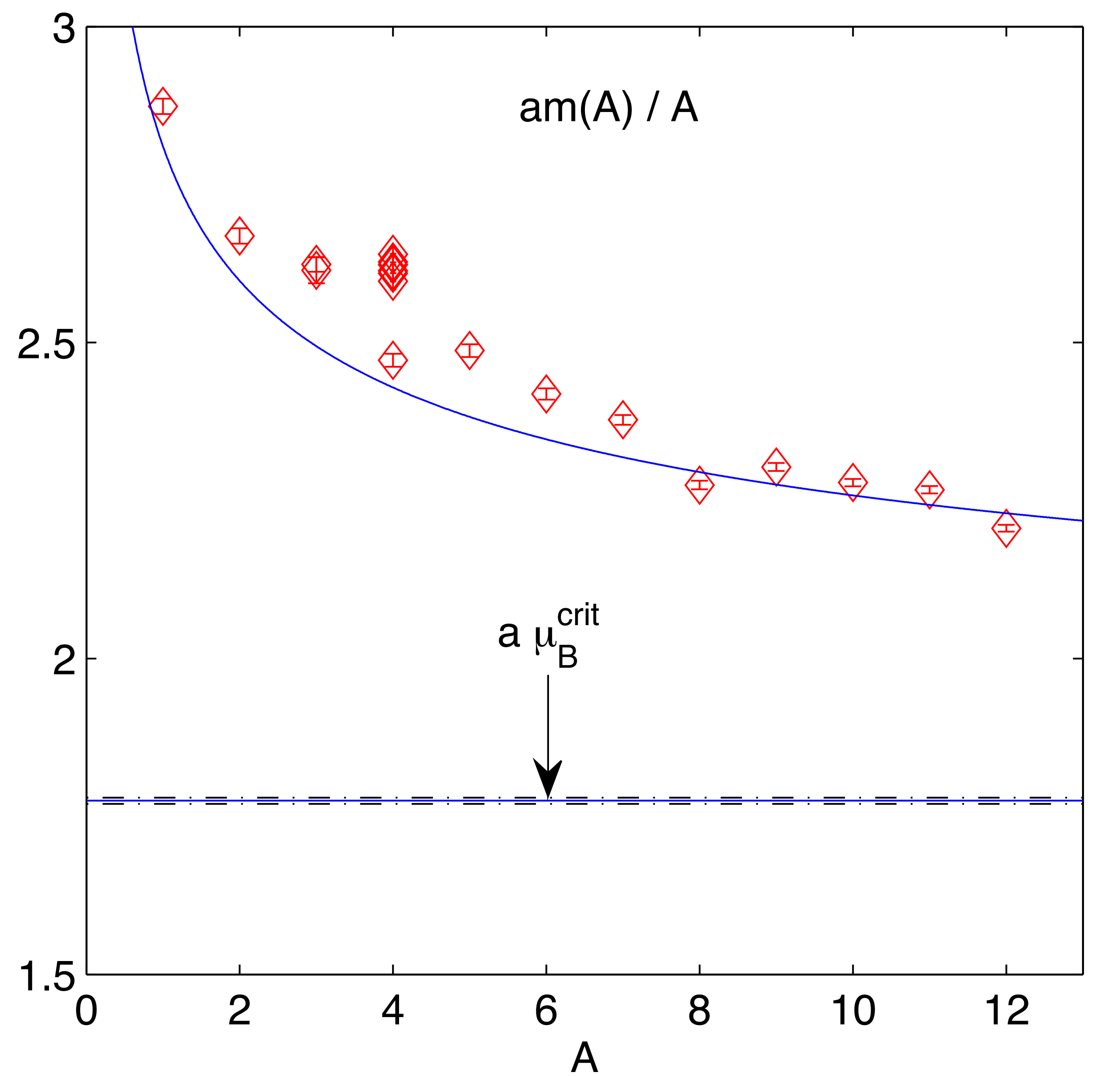


cf. Wikipedia:
($m_q \neq 0$)



Results – Crude nuclear matter: spectroscopy w/Fromm





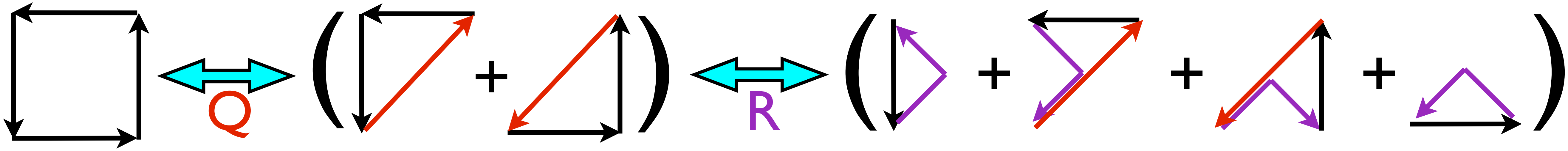
- Can compare masses of differently shaped "isotopes"
- $am(A) \sim a\mu_B^{\text{crit}} A + (36\pi)^{1/3} \sigma a^2 A^{2/3}$, ie. (bulk + surface tension)

  Bethe-Weizsäcker parameter-free (μ_B^{crit} and σ measured separately)
- "Magic numbers" with increased stability: $A = 4,\ 8,\ 12$ (reduced area)

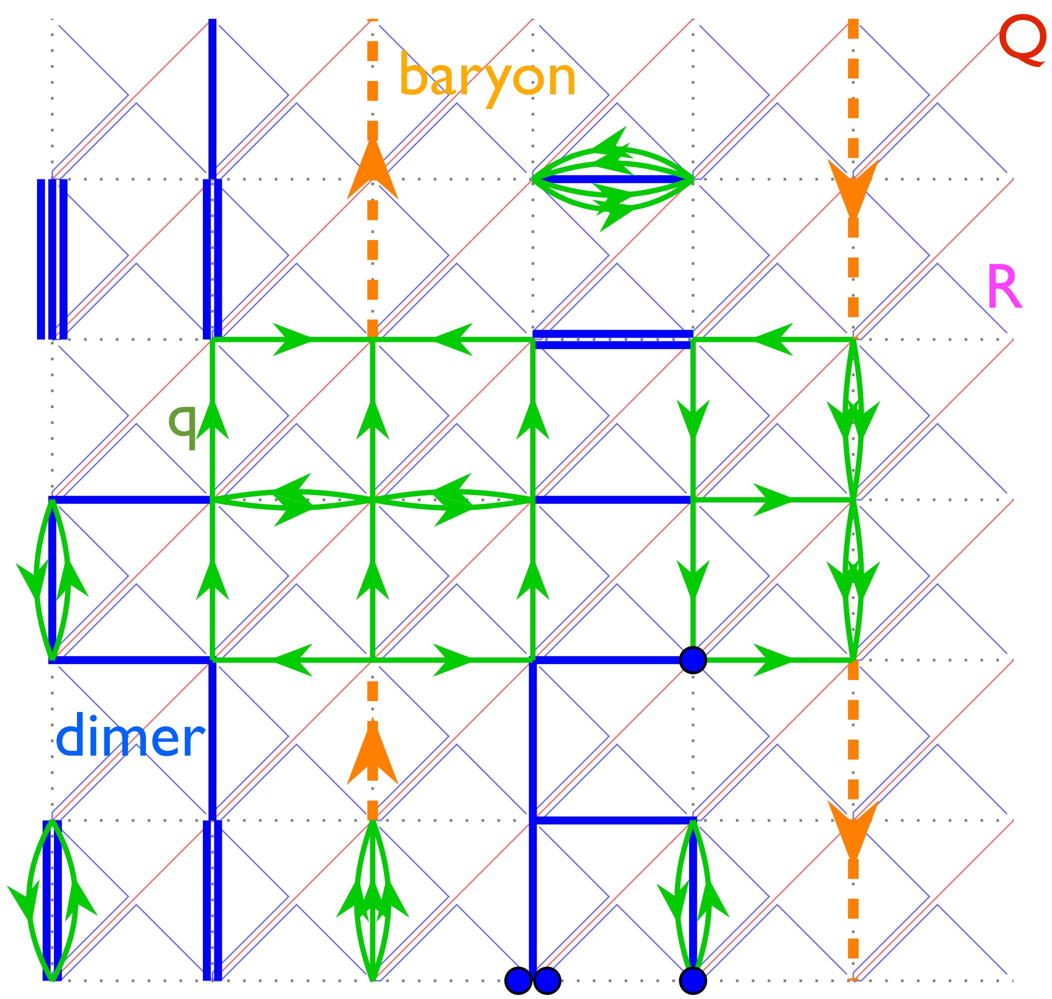
$\beta > 0$: lattice QCD with graphs

- $\beta > 0$: 4-link plaquette coupling prevents analytic link integration

decouple with Hubbard-Stratonovitch auxiliary variables Q and R



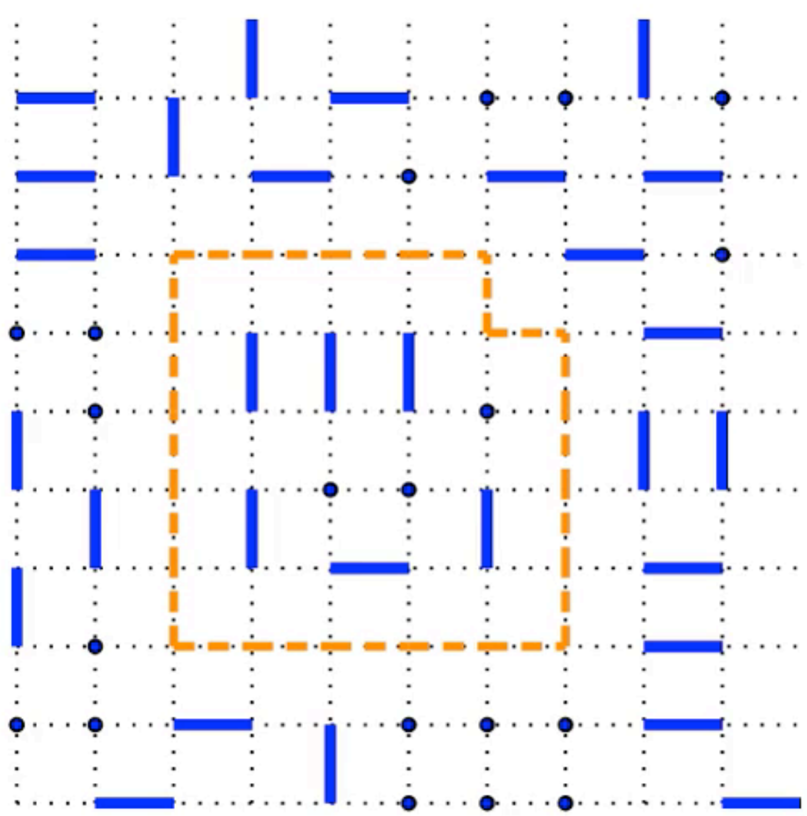
Monomers, dimers, baryons, *quarks*, all in the background of $\{Q, R\}$

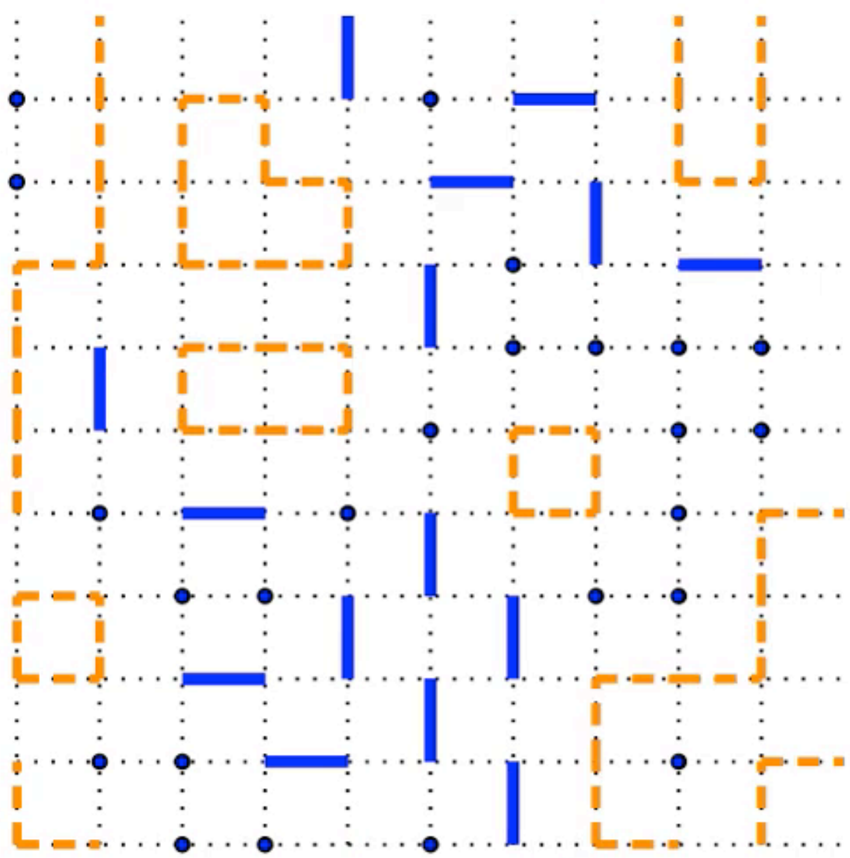


Diagrammatic Monte Carlo for 2d QED

- 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

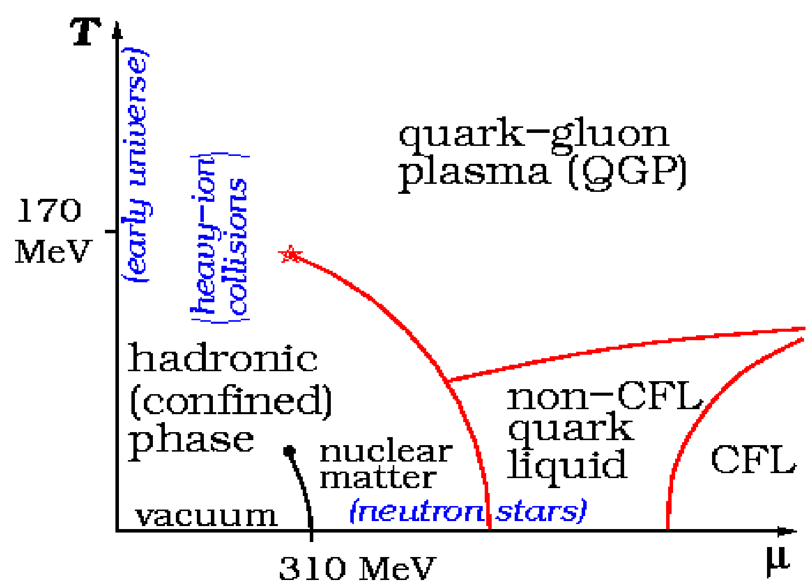


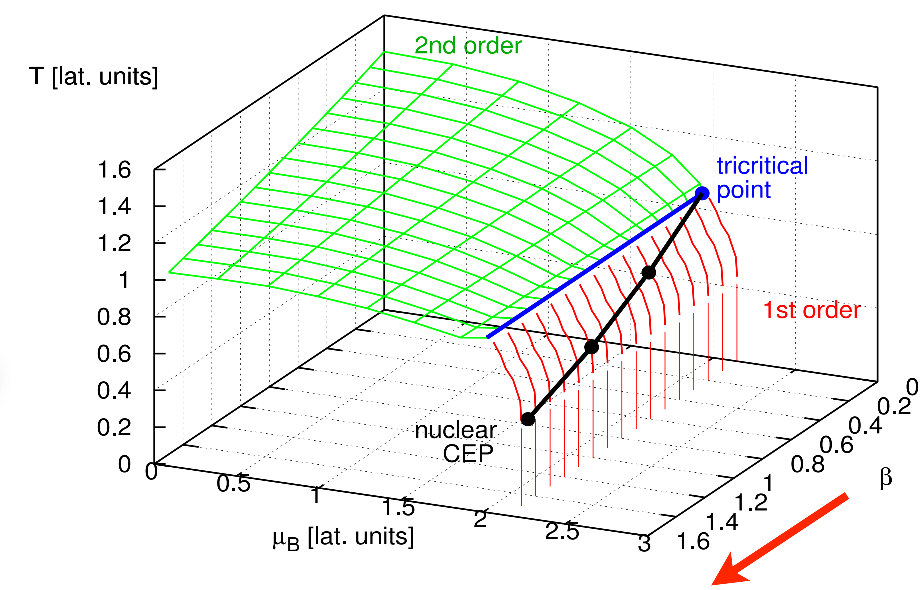


Residual sign problem? Work in progress w/Helvio Vairinhos

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 $\beta > 0$
- $U(1) \to SU(3)$
- $\mu \neq 0$





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 $\gtrsim 1/\Lambda_{\rm QCD}$

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

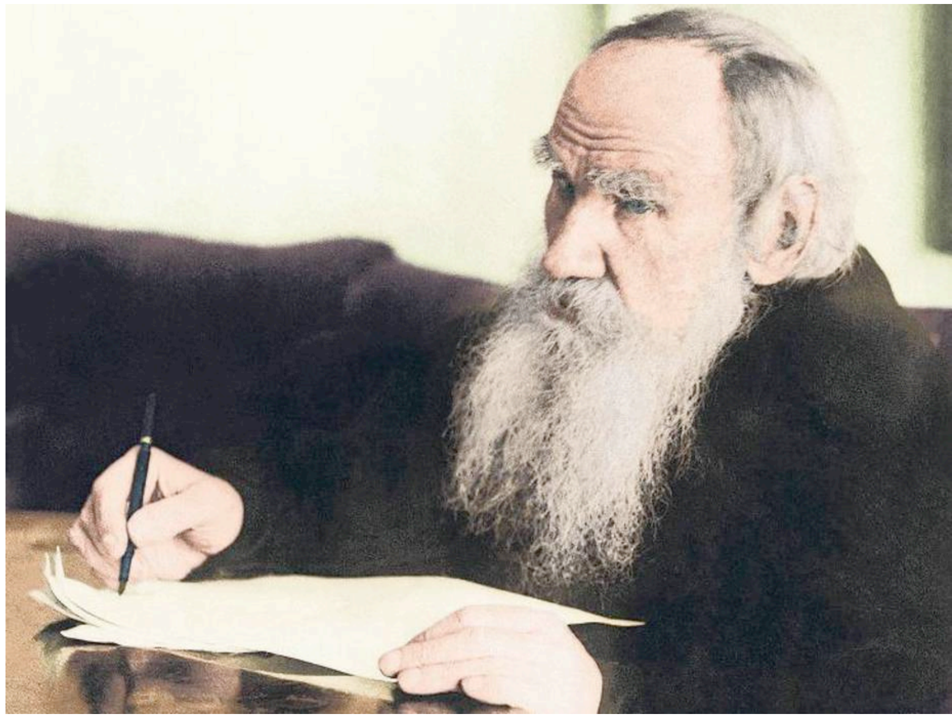
- staggered fermions $\to$ $N_f = 4$ quark flavors

Conclusions

- Tolstoi:

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

"happy" $\longrightarrow$ sign-pb free



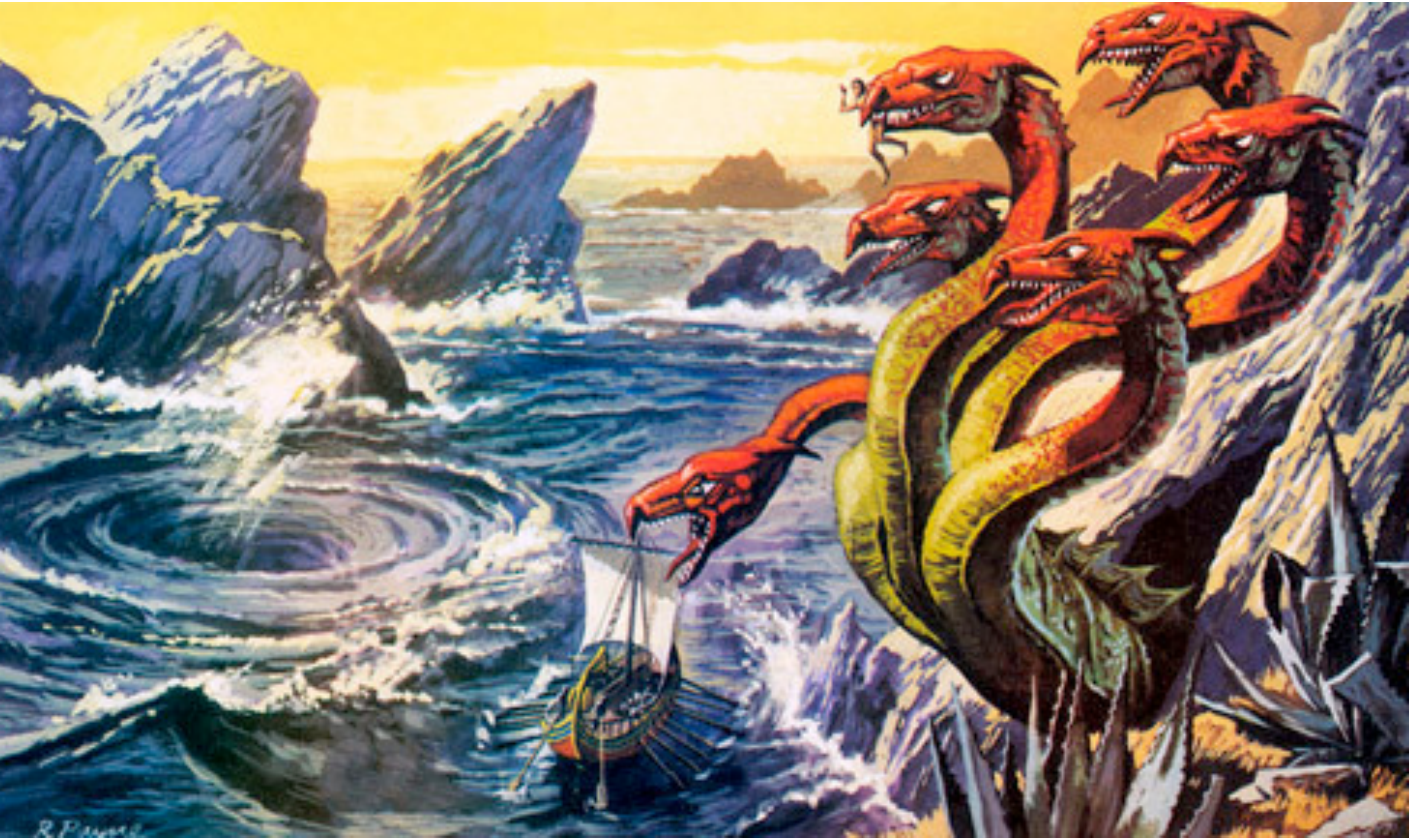
- Finite-density QCD: fermions AND bosons

still a long way to go...

Thank you for your attention

Thank you for your attention

Backup



Sign pb

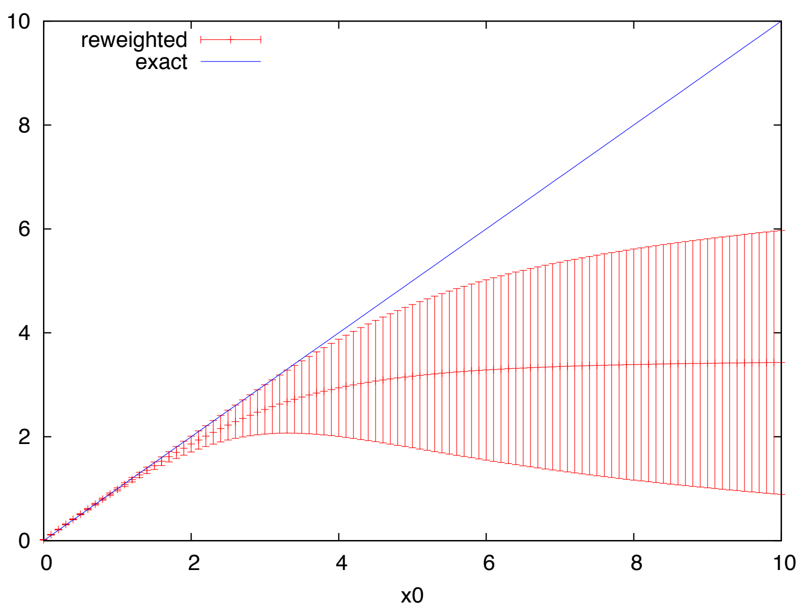
Overlap pb

More difficulties: the overlap problem

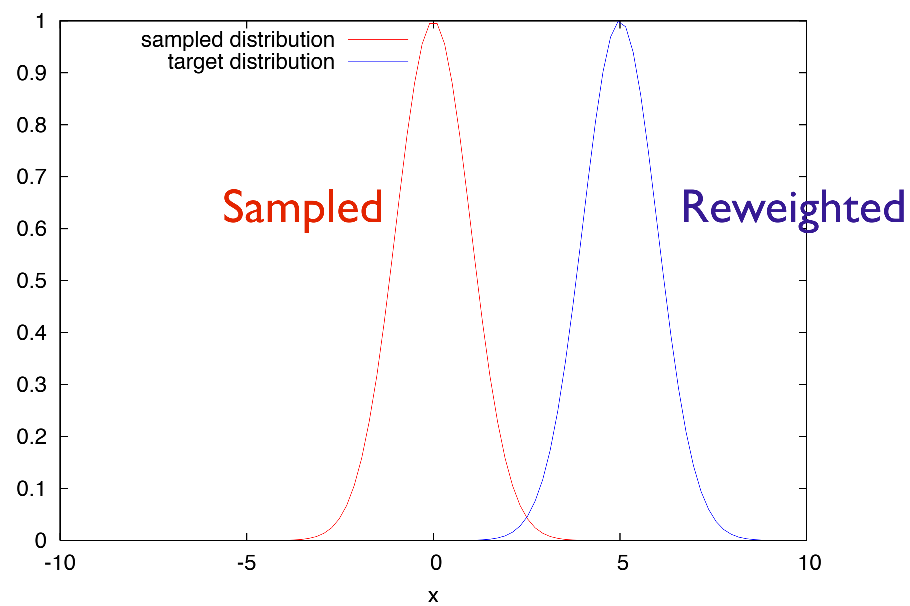
- Further danger: insufficient overlap between sampled and reweighted ensembles

> Very large weight carried by very rarely sampled states
>
> $\rightarrow$ WRONG estimates in reweighted ensemble for finite statistics

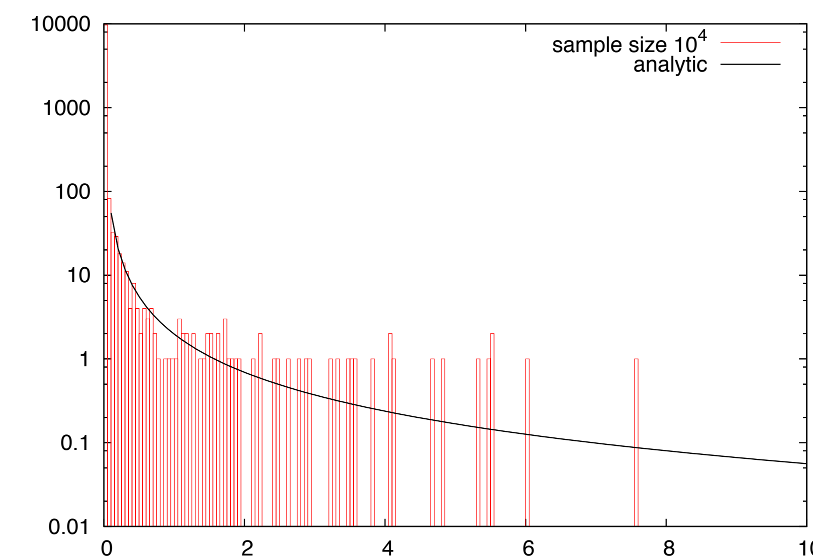
- Example: sample $\exp(-\frac{x^2}{2})$, reweight to $\exp(-\frac{(x-x_0)^2}{2}) \rightarrow \langle x \rangle = x_0$?



- Estimated $\langle x \rangle$ saturates at largest sampled x-value
- Error estimate too small



Insufficient overlap ($x_0 = 5$)



Very non-Gaussian distribution of reweighting factor

Log-normal Kaplan et al.

Solution: Need stats $\propto \exp(\Delta S)$

From QED to QCD: essential facts

	QED	QCD
Bosons:	photon	8 gluons
Fermions:	electron	quarks (up, down, strange, ..)
	Electric charge	Color charge

Confinement: quarks are bound in color-neutral hadrons: qqq baryons & $q\bar{q}$ mesons

- Baryons qqq: protons, neutrons, i.e. ordinary matter
- Mesons $q\bar{q}$: pions (lightest) and others

Nuclear interactions: residual interactions between color-neutral protons/neutrons

$\rightarrow$ Nuclear physics from first principles

Old birds: complex Langevin revival Seiler, Stamatescu, Aarts, Sexty,..

- Real action S: Langevin evolution in Monte-Carlo time τ Parisi-Wu 80's

$\frac{\partial\phi}{\partial\tau} = -\frac{\delta S[\phi]}{\delta\phi} + \eta$, 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: $\langle W\left[\phi^R + i\phi^I\right]\rangle_\tau = \frac{1}{Z}\int \mathcal{D}\phi \exp(-S[\phi]) W[\phi]$

Idea: trade oscillatory weight on real axis for positive weight in complex plane

- Gaussian example:

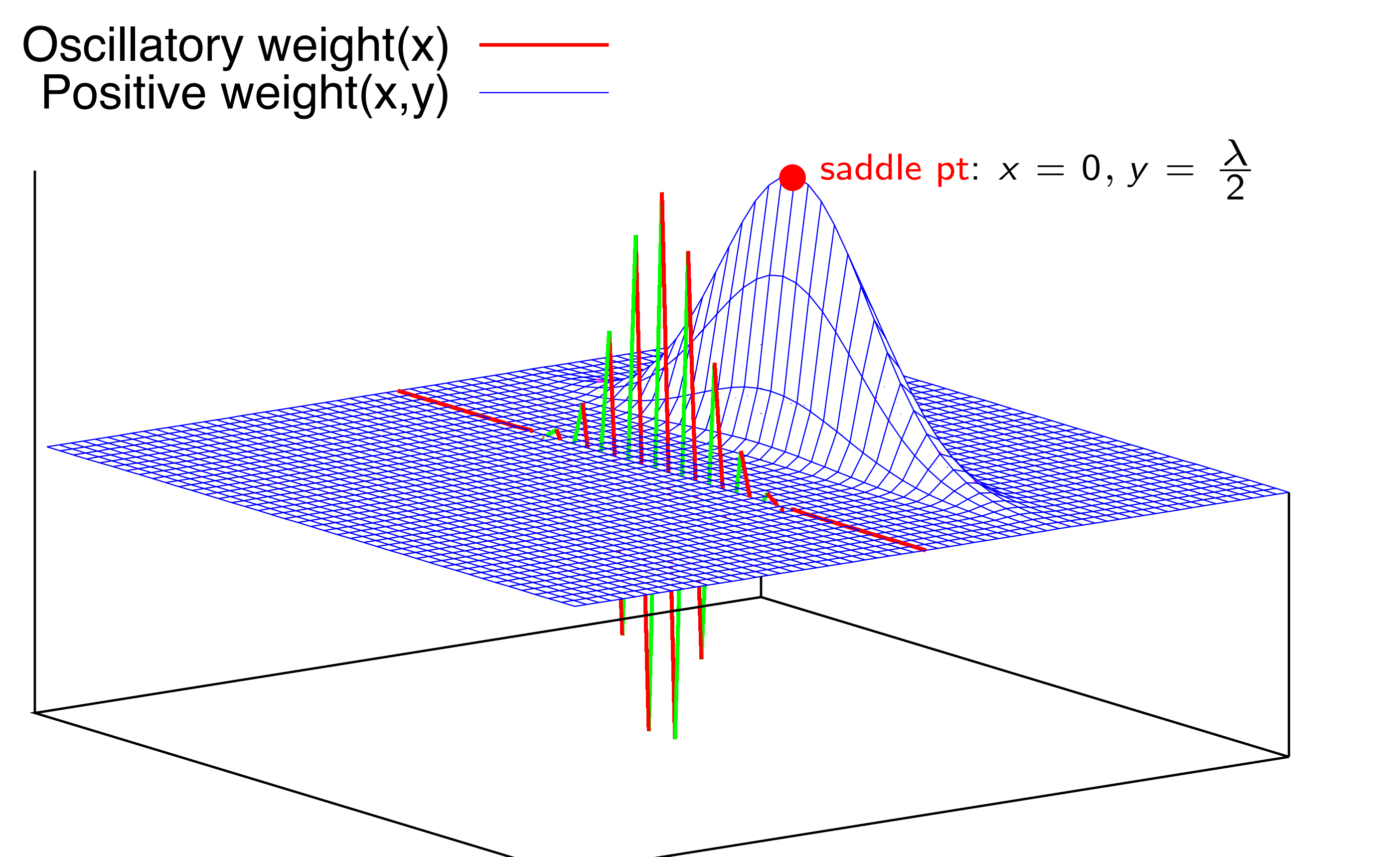
$Z(\lambda) = \int dx \exp(-x^2 + \mathbf{i}\lambda\mathbf{x})$

Complexify:

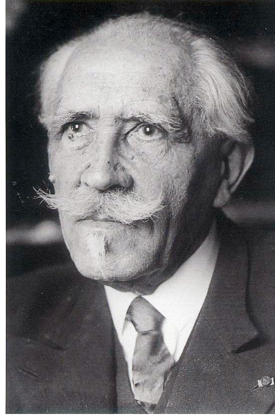
$\frac{d}{d\tau}(x + iy) = -2(x + iy) + i\lambda + \eta$

For any observable W,

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



Difficulties with complex Langevin



- Infinite set of necessary conditions to prove correctness
- Simplified: need bounded or exponentially decreasing distribution of $\mathrm{Im}(\phi)$
- Gauge invariance $\Longrightarrow$ flat directions to $\pm i\infty$ $\leftarrow$ "gauge cooling"?

- Convergence lost when noise is made complex

- Action is analytically continued: $S = S_{YM} + \log \det \not{D}$

how to deal with cut in log det $\not{D}$? with log singularity when det $\not{D} = 0$??

Caveat:

Complex Langevin gives wrong answer when system is too disordered, also when there is no sign pb! $3d$ XY model, Aarts & James, 1005.3468

Robustness?

Importance of classical stationary points + fluctuations Guralnik & Pehlevan

New bird: Lefschetz thimble

- Same starting point as complex Langevin:

  analytic continuation in complexified space

- Follow steepest ascent from action minima $\rightarrow$ constant $\mathrm{Im}(S)$

The weights of all configurations along a thimble have [almost] the same phase

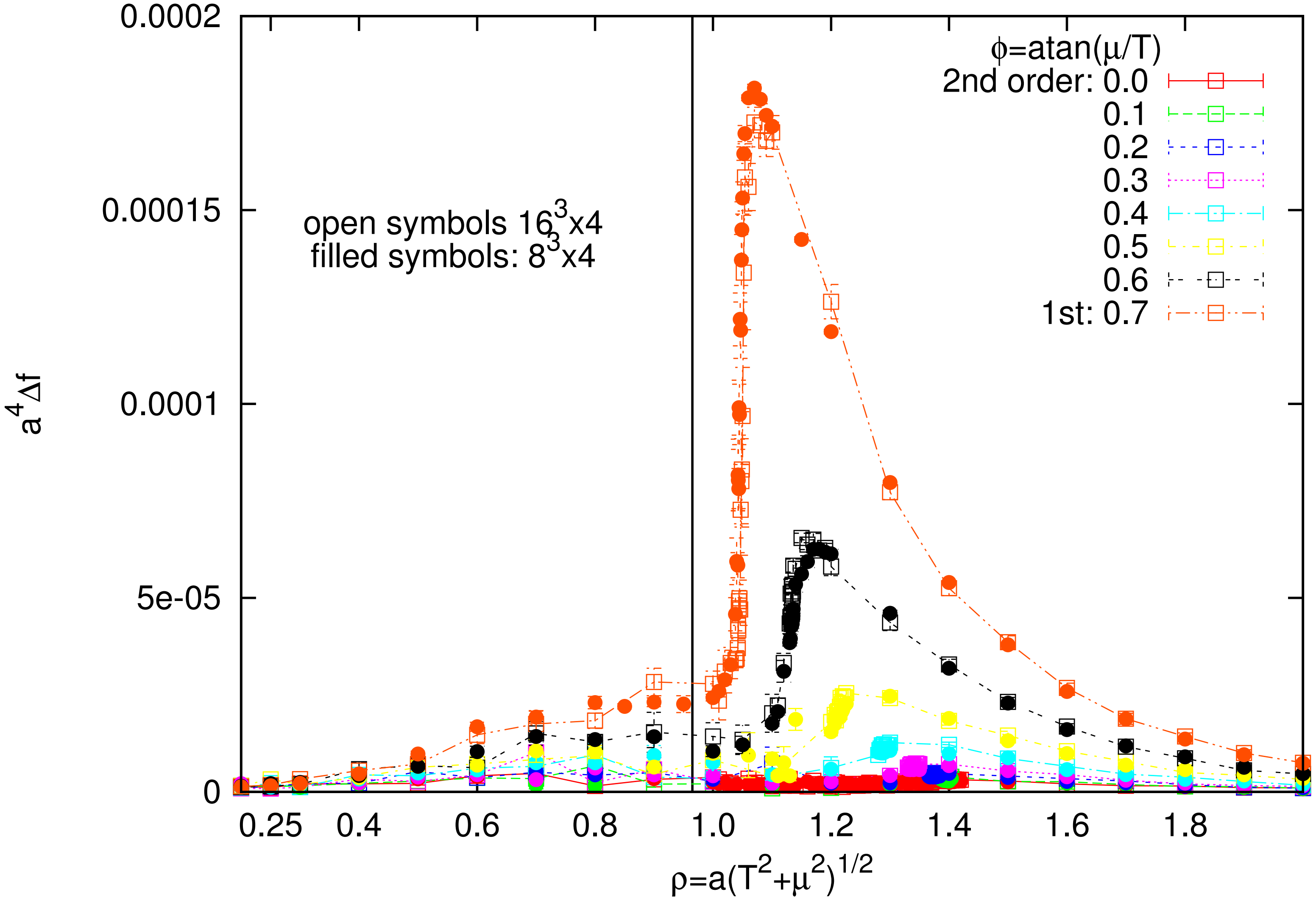
- Problems: - find the many (?) thimbles

  - control their phase cancellations

  - deal with non-analyticities of S

Under construction

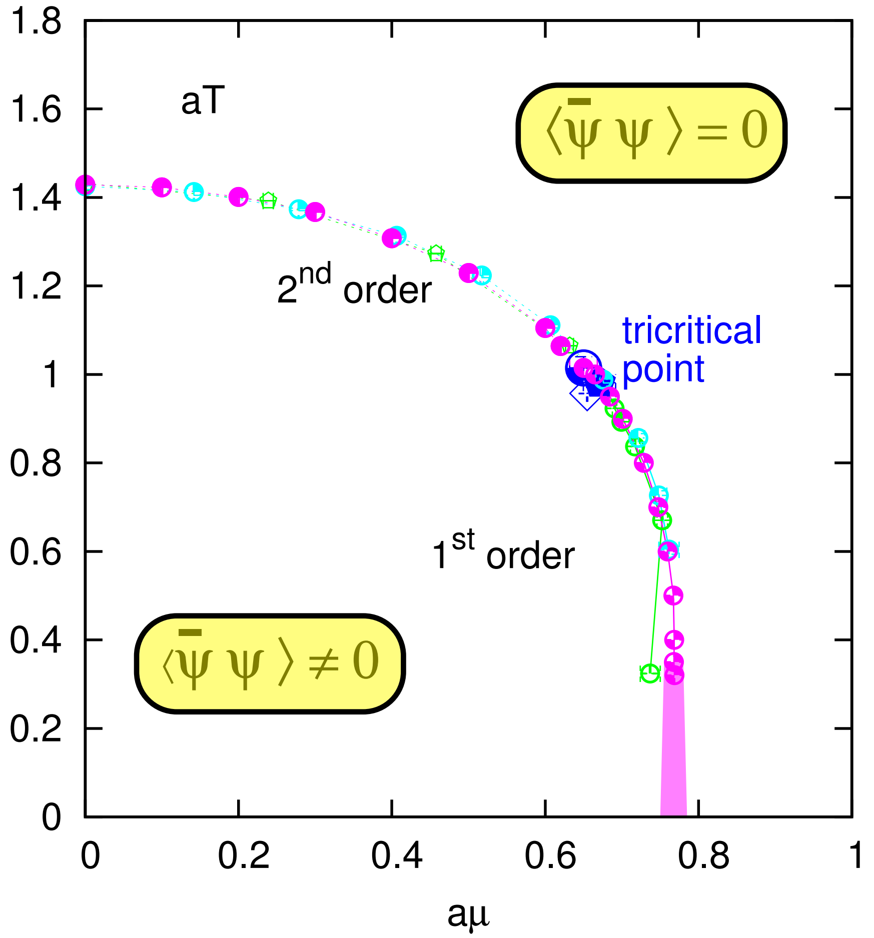
Severity of sign problem? Monitor $\Delta f = -\frac{1}{V}\log\langle \text{sign}\rangle$



- $\langle \text{sign}\rangle = \frac{Z}{Z_{||}} \sim \exp(-\frac{V}{T}\Delta f(\mu^2))$ 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 ($m_q = 0$)

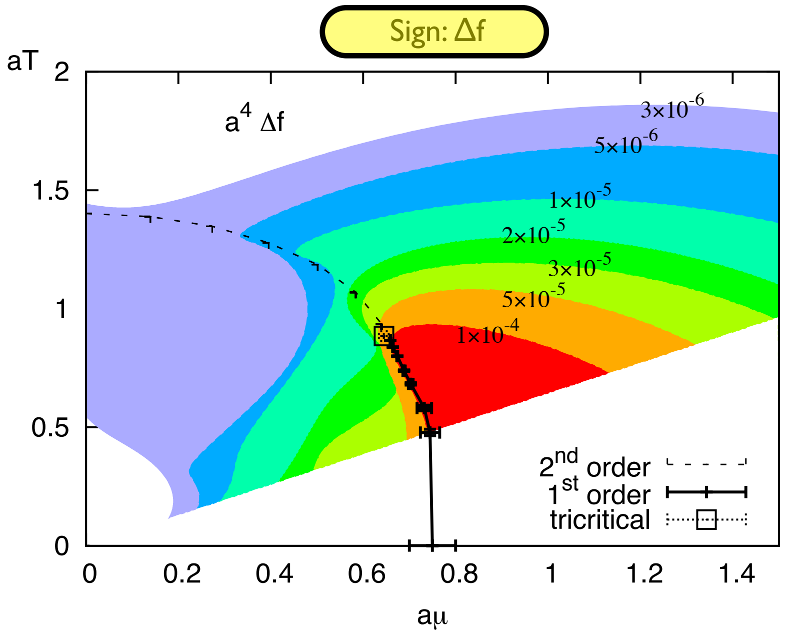
w/Unger, Langelage, Philipsen

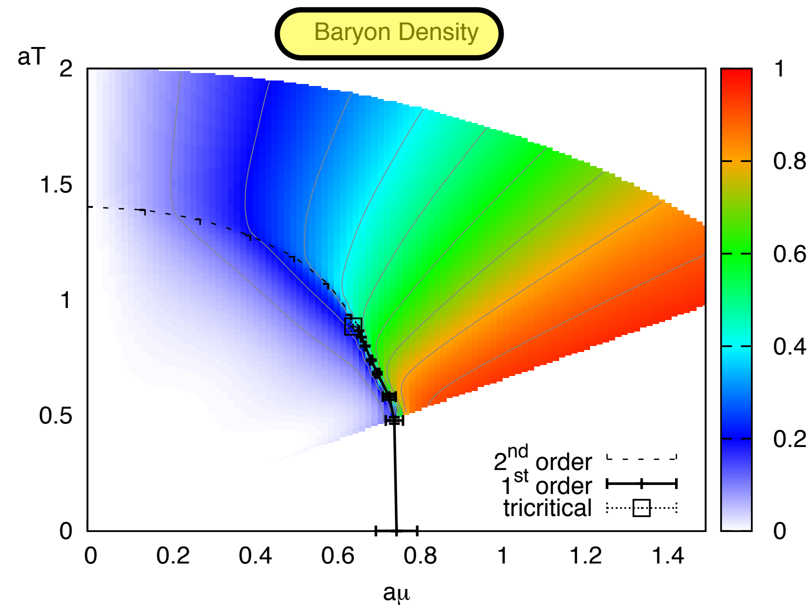


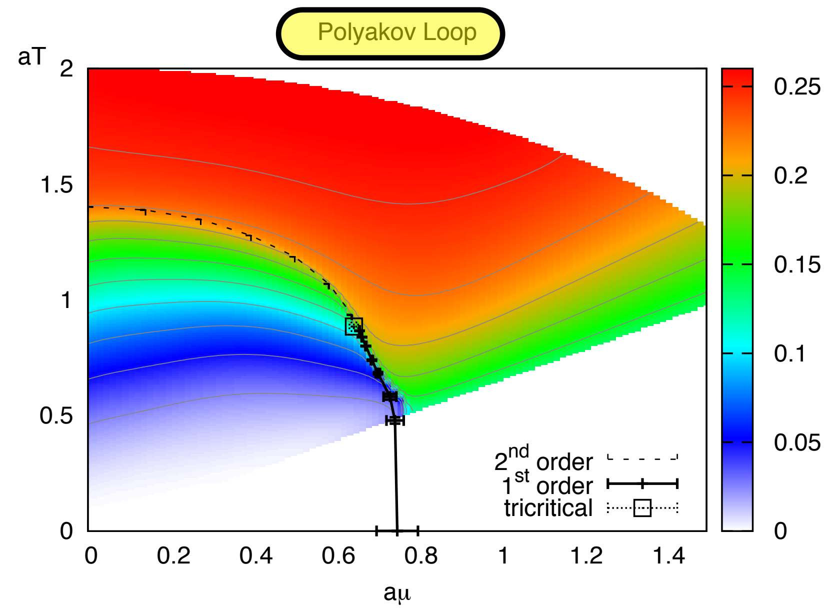
- Chiral phase transition ($m_q = 0$):

2nd → 1rst order as μ increases: *tricritical* point

- Finite-N_t corrections → continuous-time
- Baryon density jumps at 1rst-order transition
- Polyakov loop changes at chiral transition







Moving from $\beta = 0$ toward the continuum limit $\beta \to +\infty$

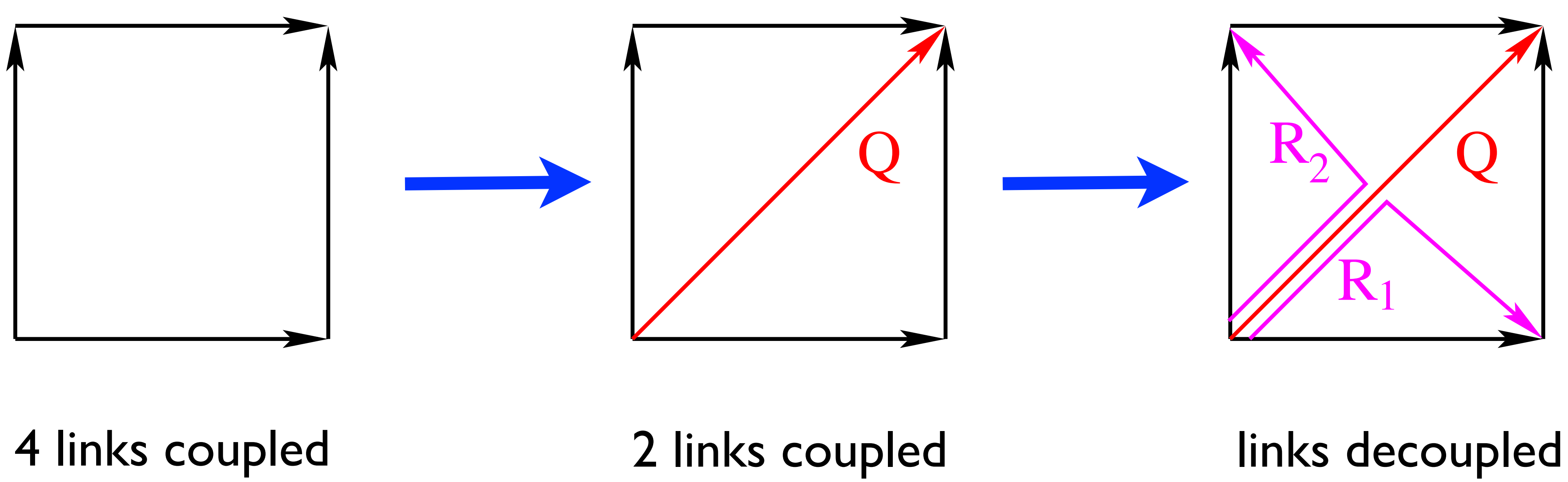
- $\beta = 0$: gauge links U are not directly coupled to each other:

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

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 transformations



Moving from $\beta = 0$ toward the continuum limit $\beta \to +\infty$

Simple: $\mathcal{O}(\beta)$ approximation

- 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 $\{q_P\} \ \to$ exact at $\mathcal{O}(\beta)$ 1406.4397 $\to$ PRL

More ambitious: arbitrary β

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

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

Product of 1-link integrals performed analytically

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

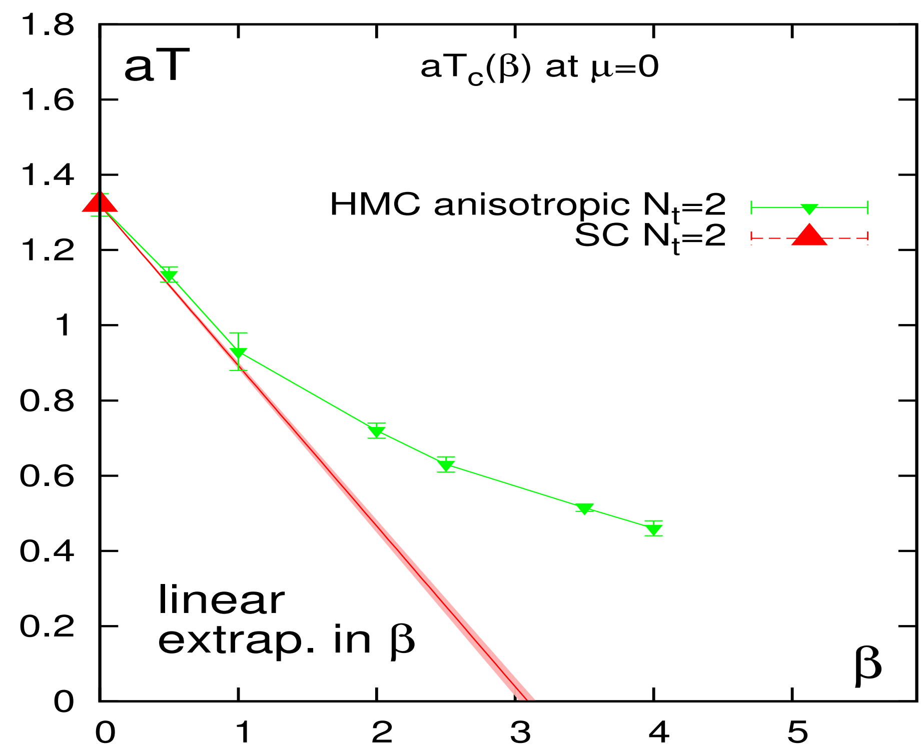
Decouple gauge links by Hubbard-Stratonovich transformations

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 $\{q_P\}$ → exact at $\mathcal{O}(\beta)$
- $q_P = 1$ → 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 $\to$ PRL

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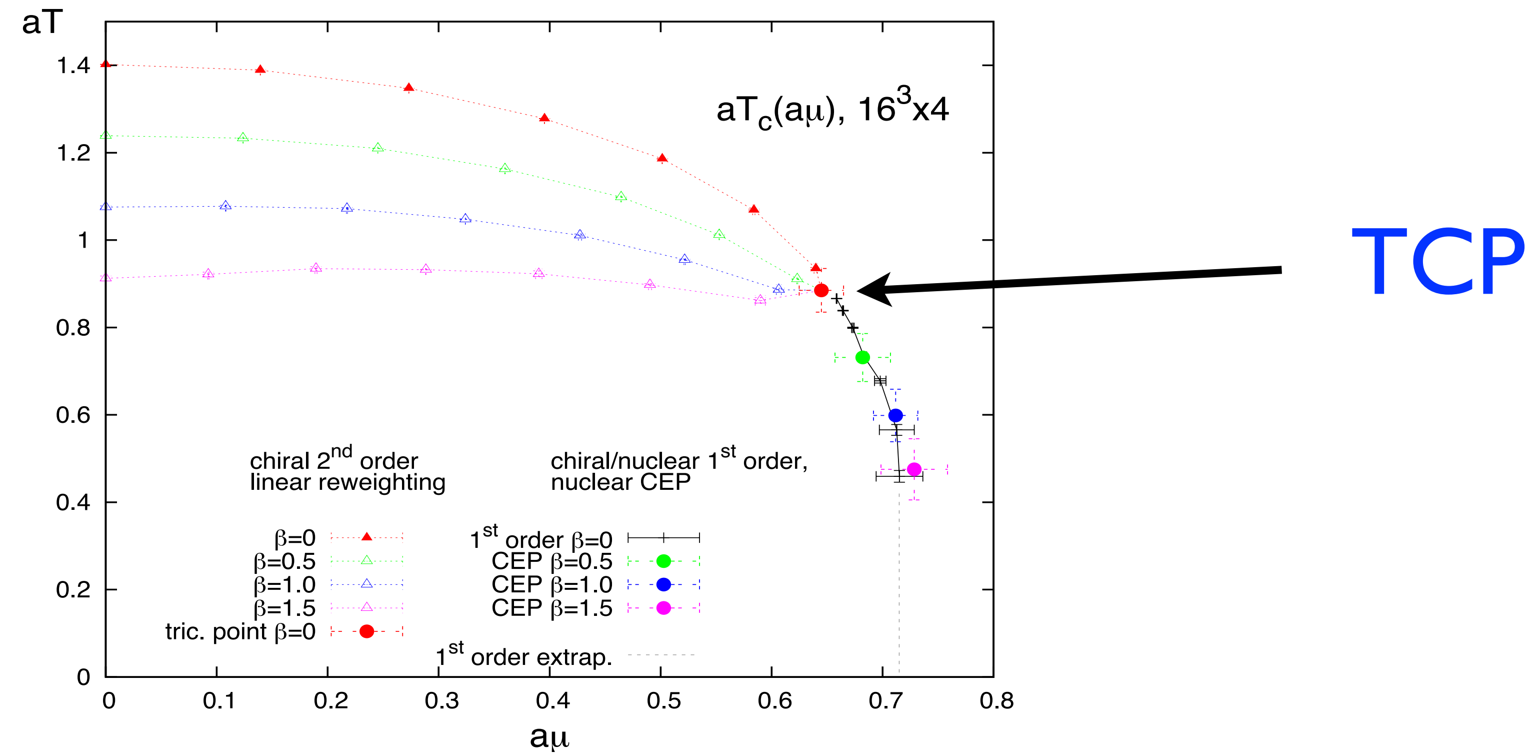

- $\mu = 0$: crosscheck with HMC ok; linear (aT_c) extrapolation good up to $\beta \sim 1$
- $\mu \neq 0$: - phase boundary more "rectangular" with TCP at corner

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

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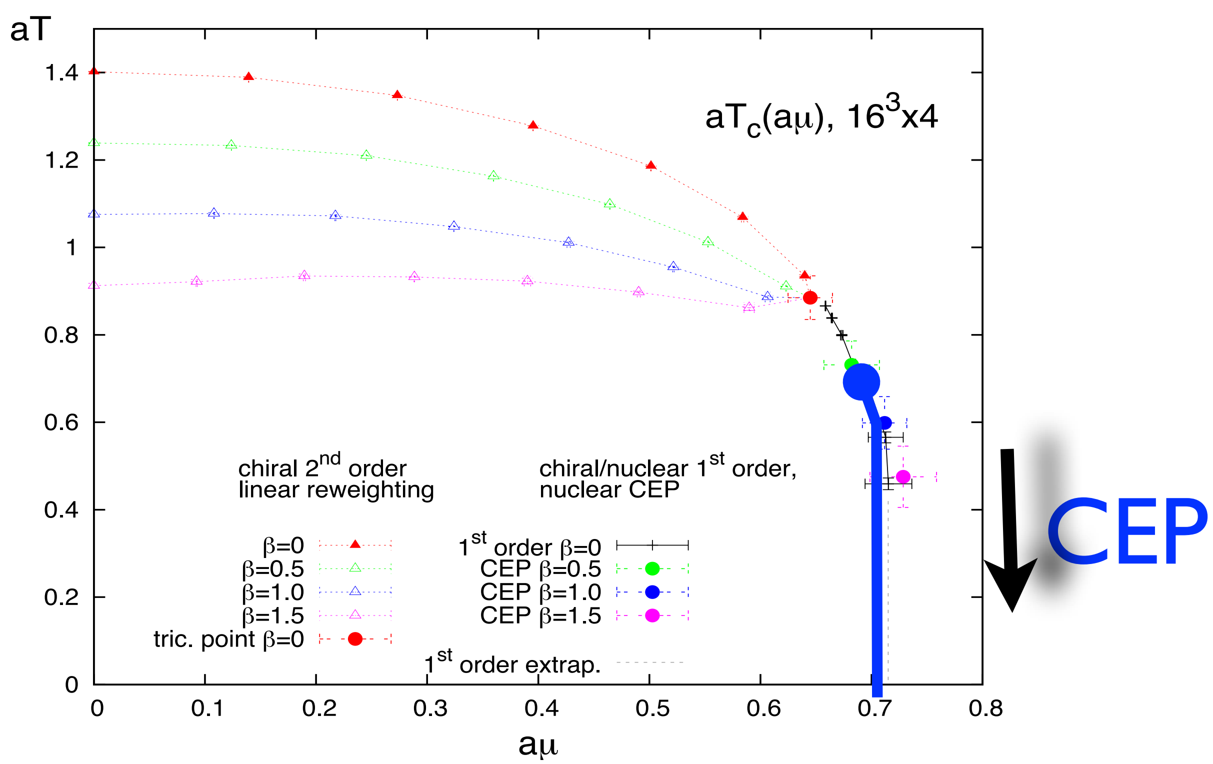
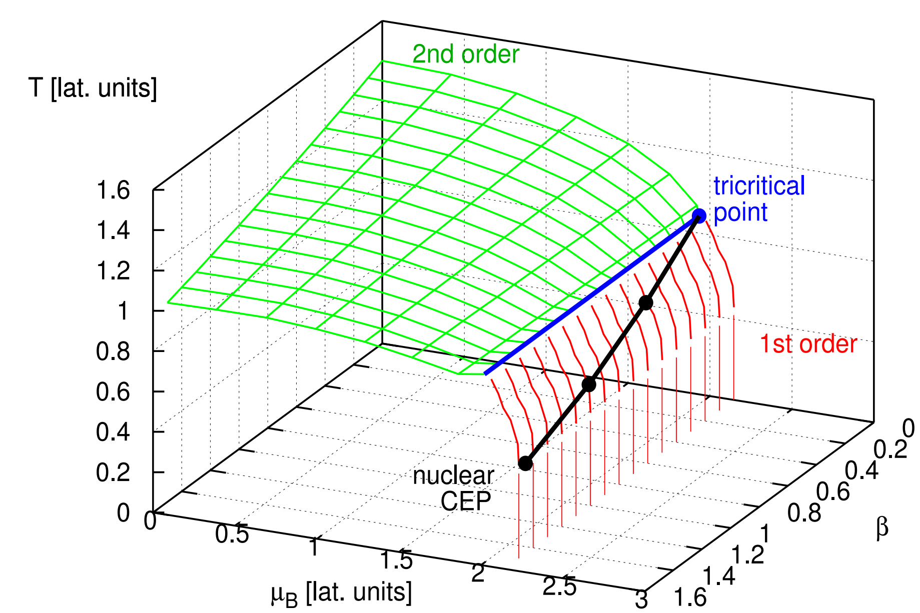




- $\mu = 0$: crosscheck with HMC ok; linear (aT_c) extrapolation good up to $\beta \sim 1$
- $\mu \neq 0$: - phase boundary more "rectangular" with TCP at corner
  - liquid-gas CEP splits and moves down ?

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

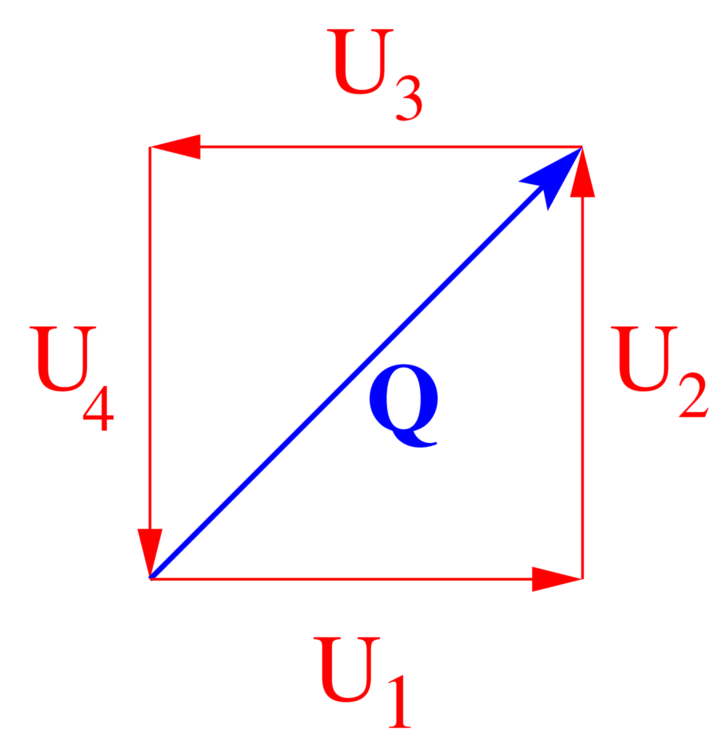
Decouple gauge links by Hubbard-Stratonovich transformation:

Hubbard-Stratonovich variant:

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

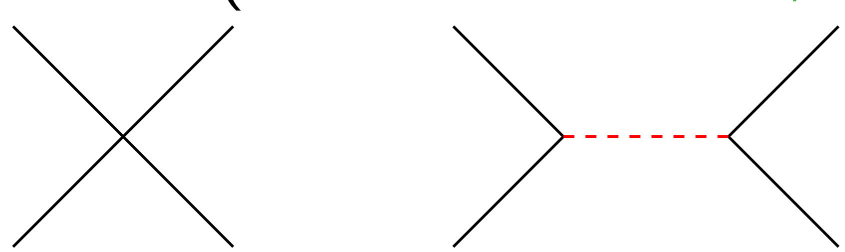
$$\Updownarrow$$

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



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

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

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

Vairinhos & PdF, 1409.8442

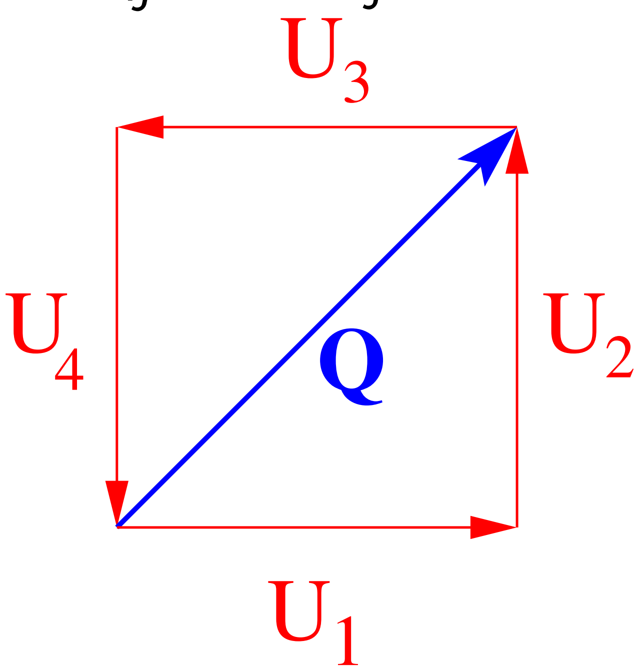
- Hubbard-Stratonovich: $\forall Y \in \mathbf{C}^{N\times N}$, $e^{\mathrm{Tr}\,Y^\dagger Y} = \mathcal{N}\int dX\ e^{\mathrm{Tr}(X^\dagger Y + XY^\dagger)}$

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

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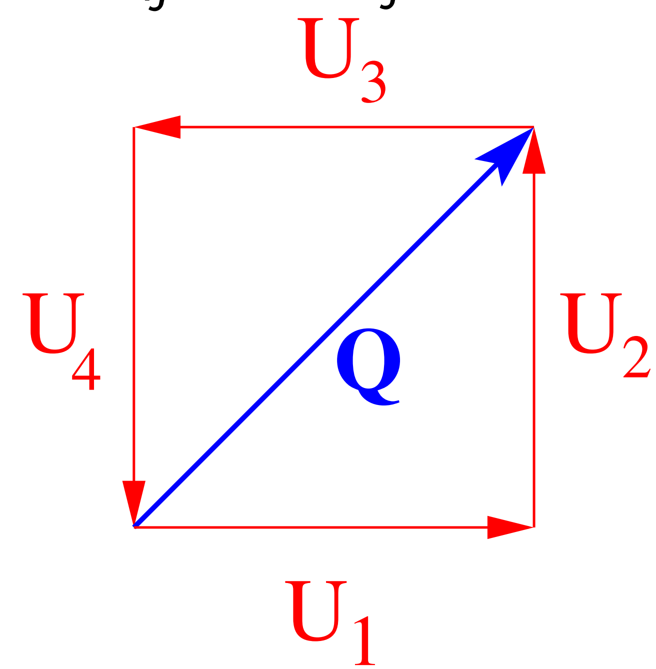
$$Y = (U_1 U_2 + U_4^\dagger U_3^\dagger),\; X = Q$$

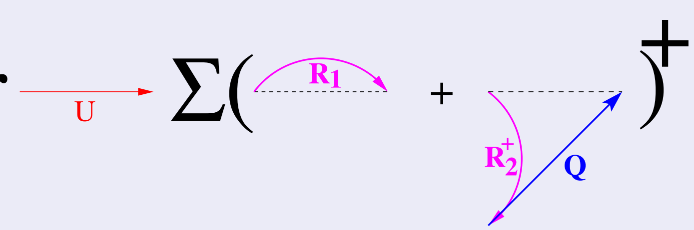
$$S_{2-\mathrm{link}} = \mathrm{ReTr}\; Q^\dagger (U_1 U_2 + U_4^\dagger U_3^\dagger)$$

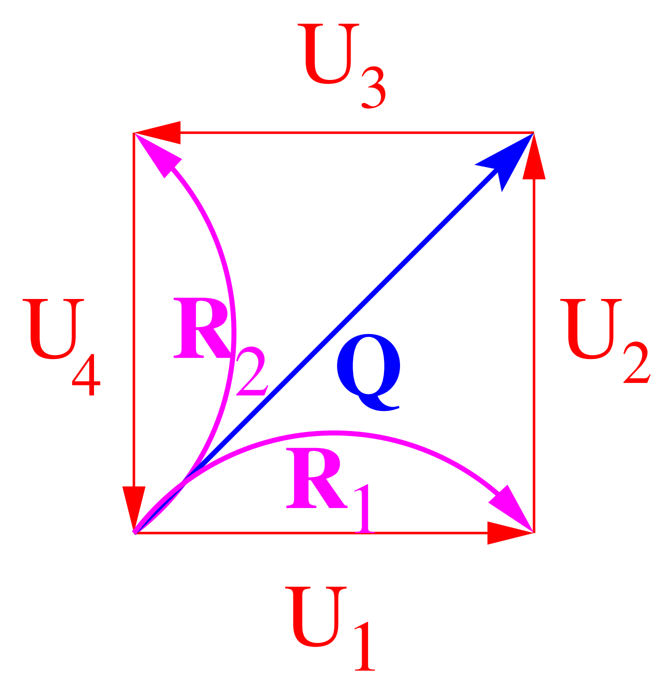


- 2 → 1-link action:

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

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





2-link action → 1-link → 0-link

Vairinhos & PdF, 1409.8442

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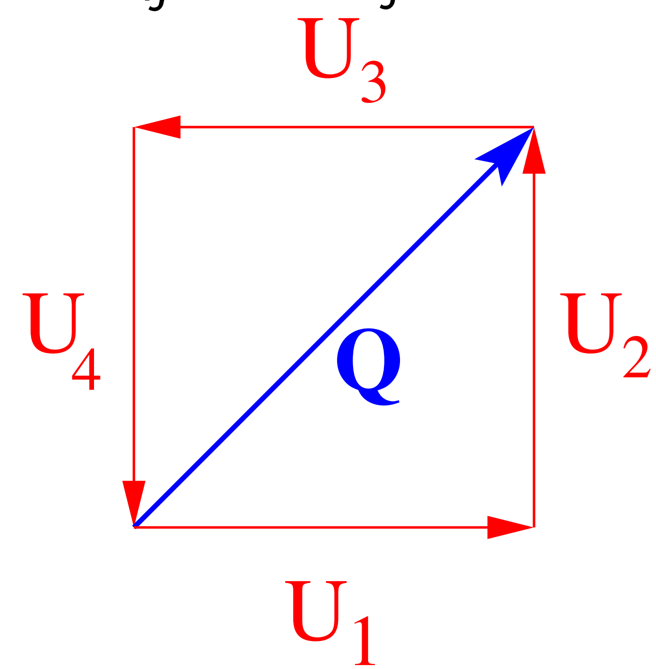
where $X \in \mathbf{C}^{N\times N}$ with Gaussian measure $dX \propto \prod_{ij} dx_{ij} dx_{ij}^* e^{-|x_{ij}|^2}$

- 4 → 2-link action:

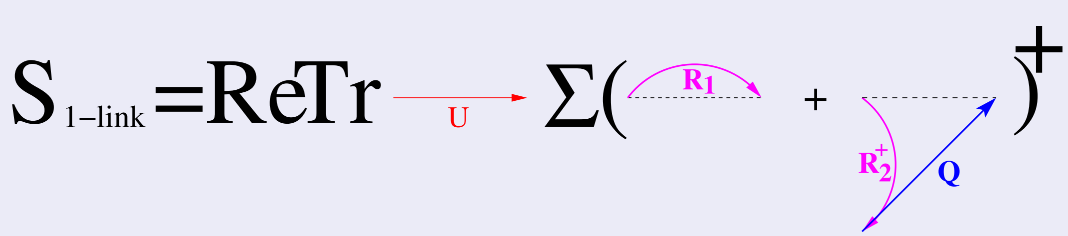
$$Y = (U_1 U_2 + U_4^\dagger U_3^\dagger), \; X = Q$$

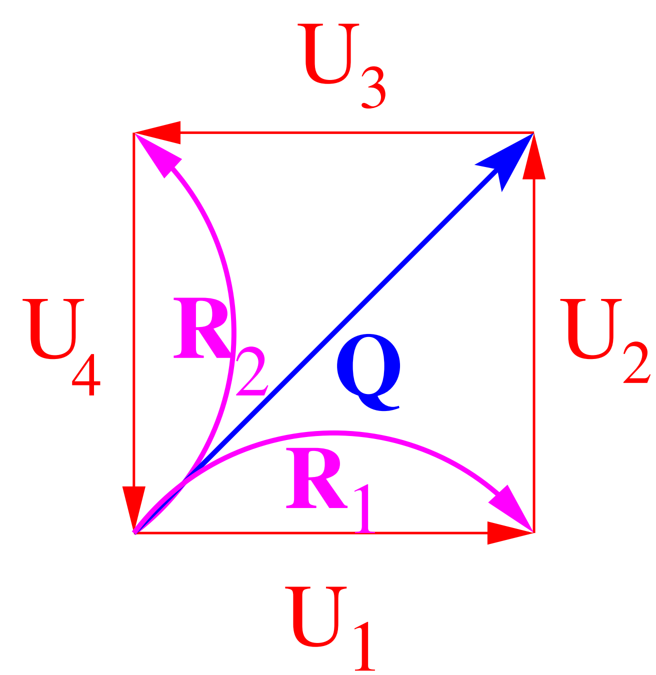
$$S_{2-\mathrm{link}} = \mathrm{ReTr} \; Q^\dagger (U_1 U_2 + U_4^\dagger U_3^\dagger)$$



- 2 → 1-link action:

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

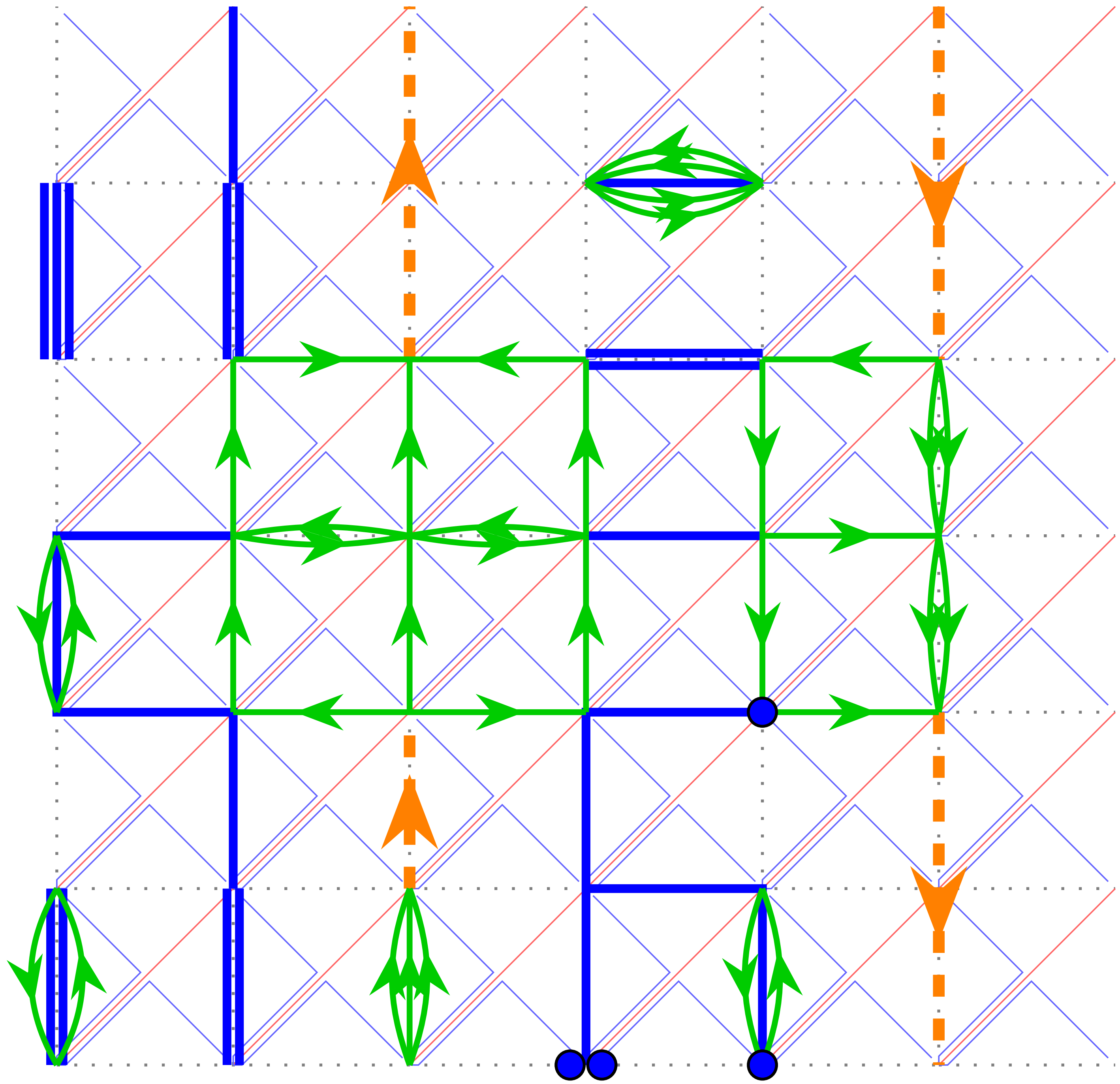




- 1 → 0-link action: integrate out U analytically – *also with fermion sources*

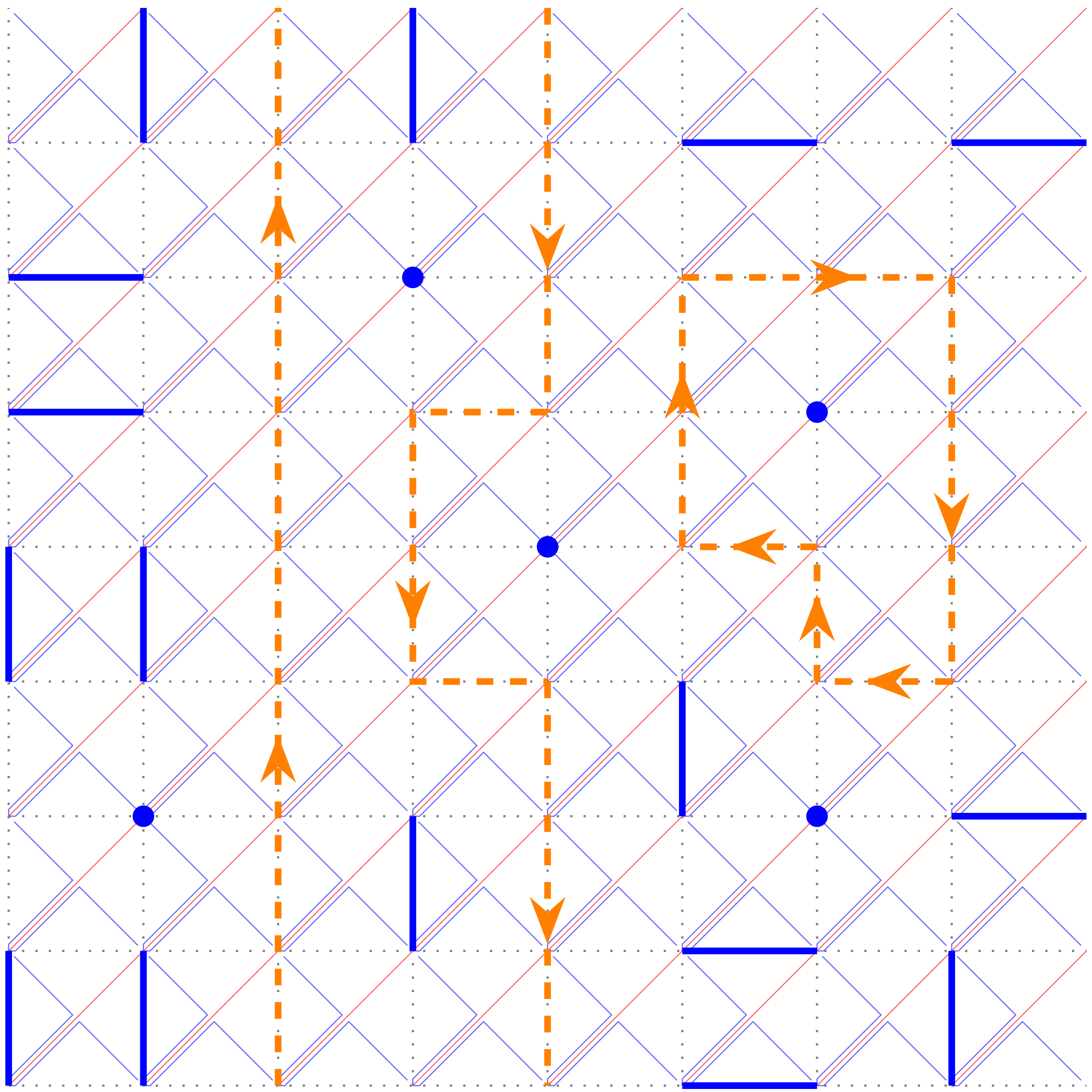
QCD with graphs

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



Start with a simpler case: 2d QED

$\beta > 0 \;\rightarrow\;$ Monomers, dimers, electron loops, in the background of $\{Q, R\}$



Start with a simpler case: 2d QED

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

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

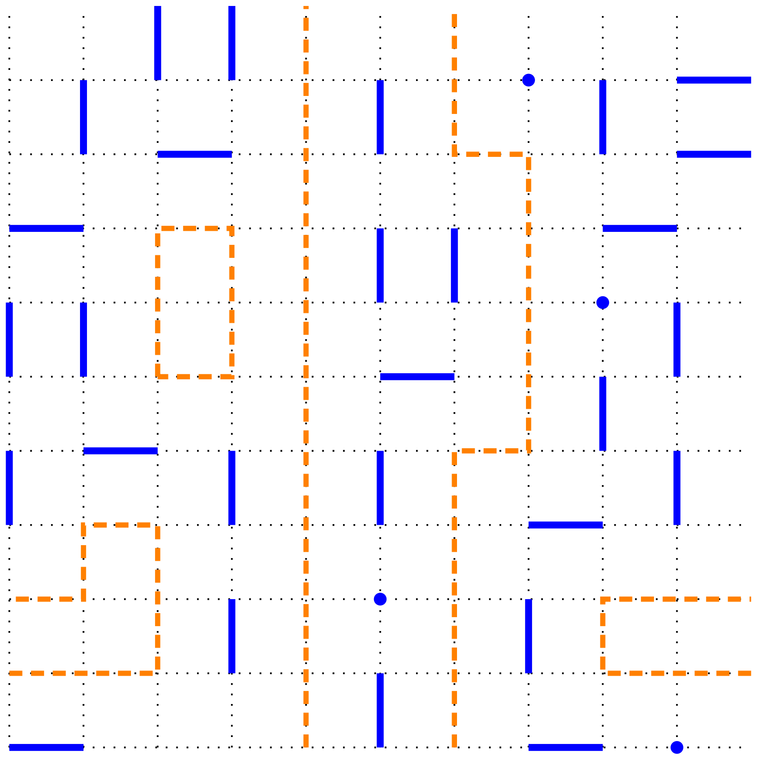
$$=\int\mathcal{G}_\beta[Q,R]\prod_{x,\mu}I_0(\beta|J_{x\mu}|)\sum_{\{n,k,C\}}\left(\prod_x(2am)^{n_x}\right)\left(\sigma_F(C)\prod_{i=1}^{\#C}2\,\mathrm{Re}(W(C))\right)$$

i.e. monomers, dimers and electron loops

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

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

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



Start with a simpler case: 2d QED

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

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

i.e. monomers, dimers (weight 1) and electron loops

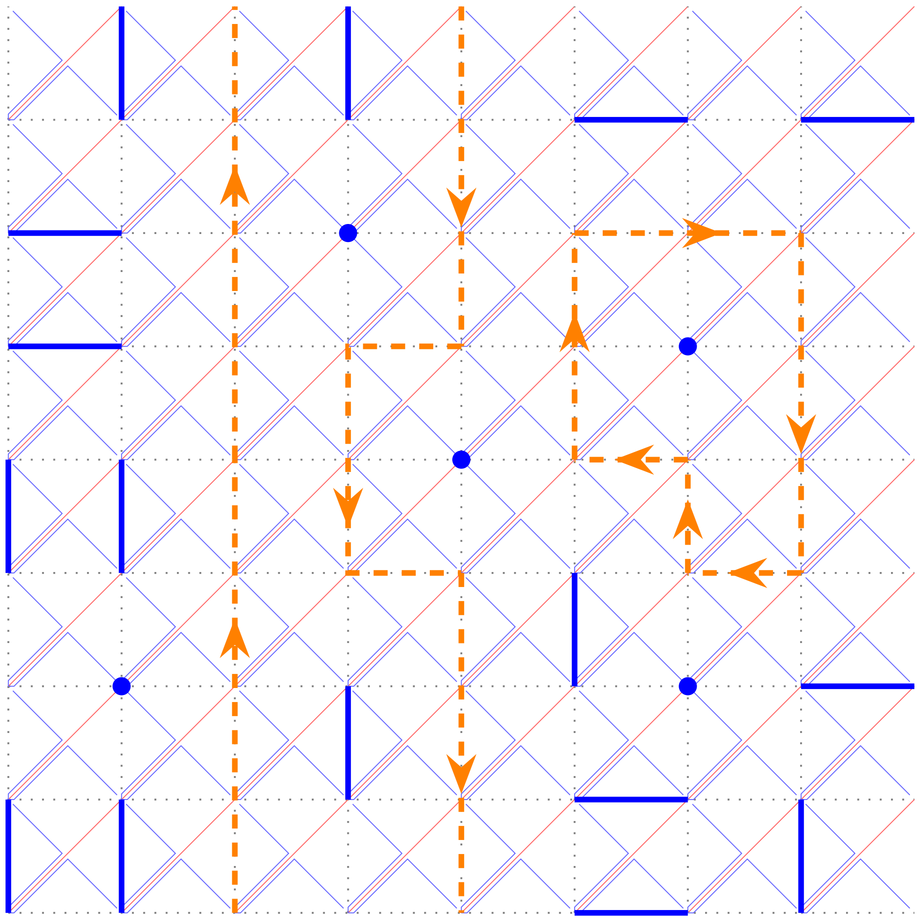
- Careful: weight of electron loop is *global* and can be *negative*

$\sigma_F(C) = \pm 1$ depends on loop geometry

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

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

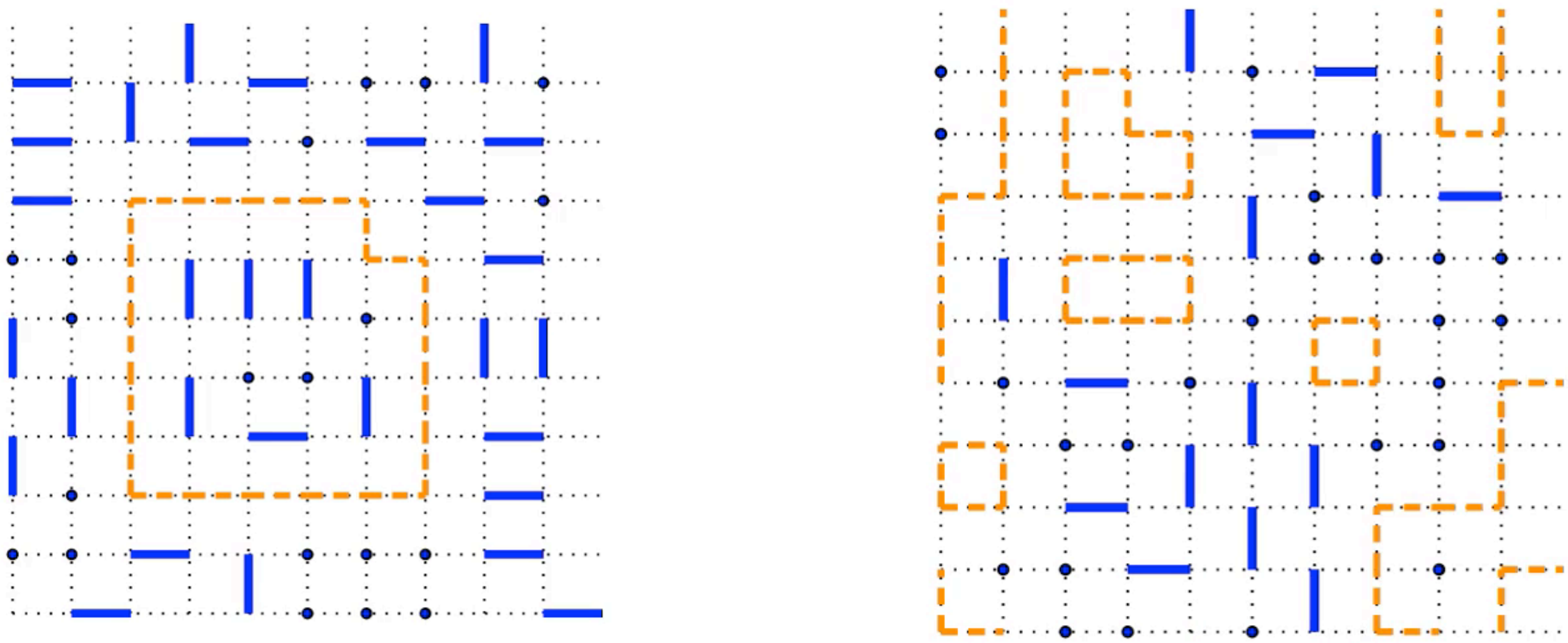
phase factor



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

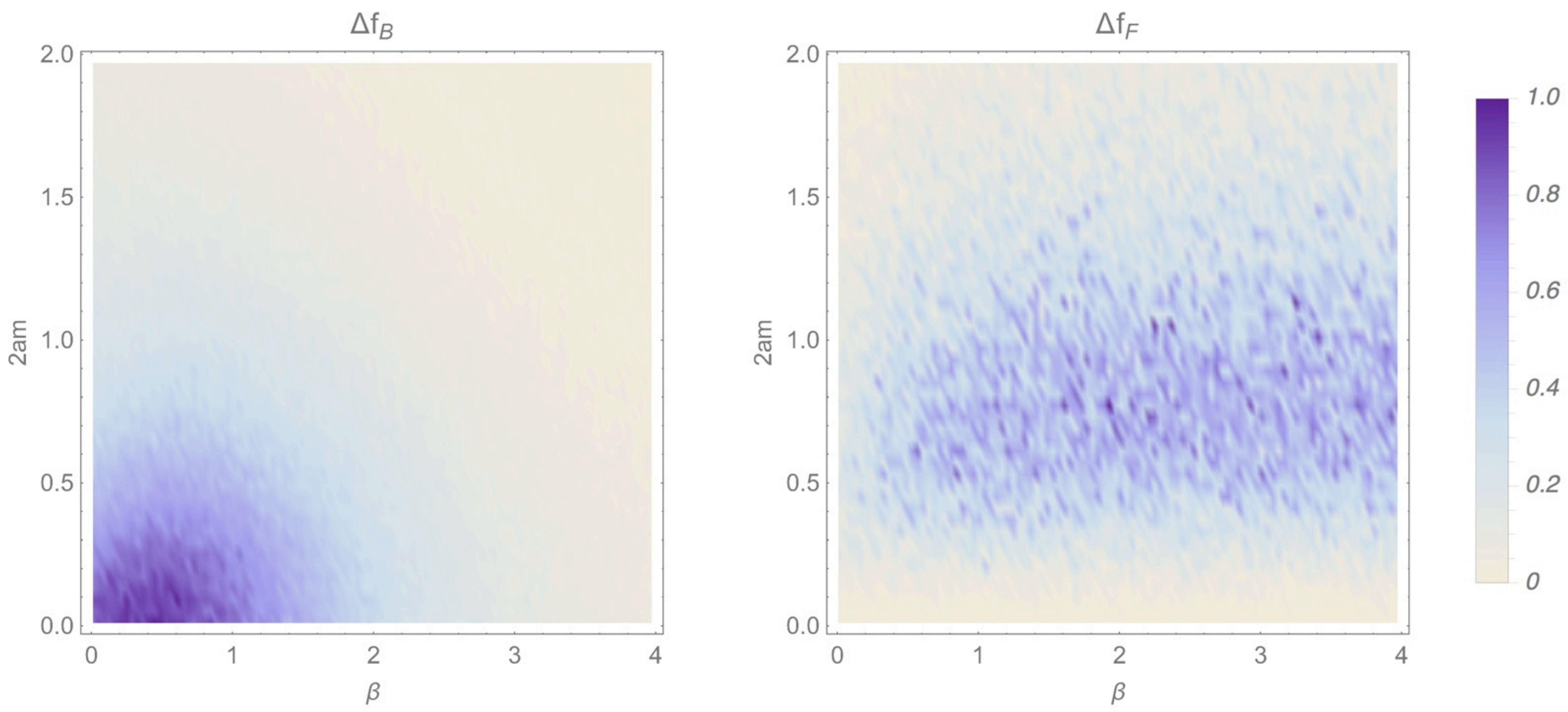


Residual sign problem? Work in progress w/Helvio Vairinhos

Sign problems

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

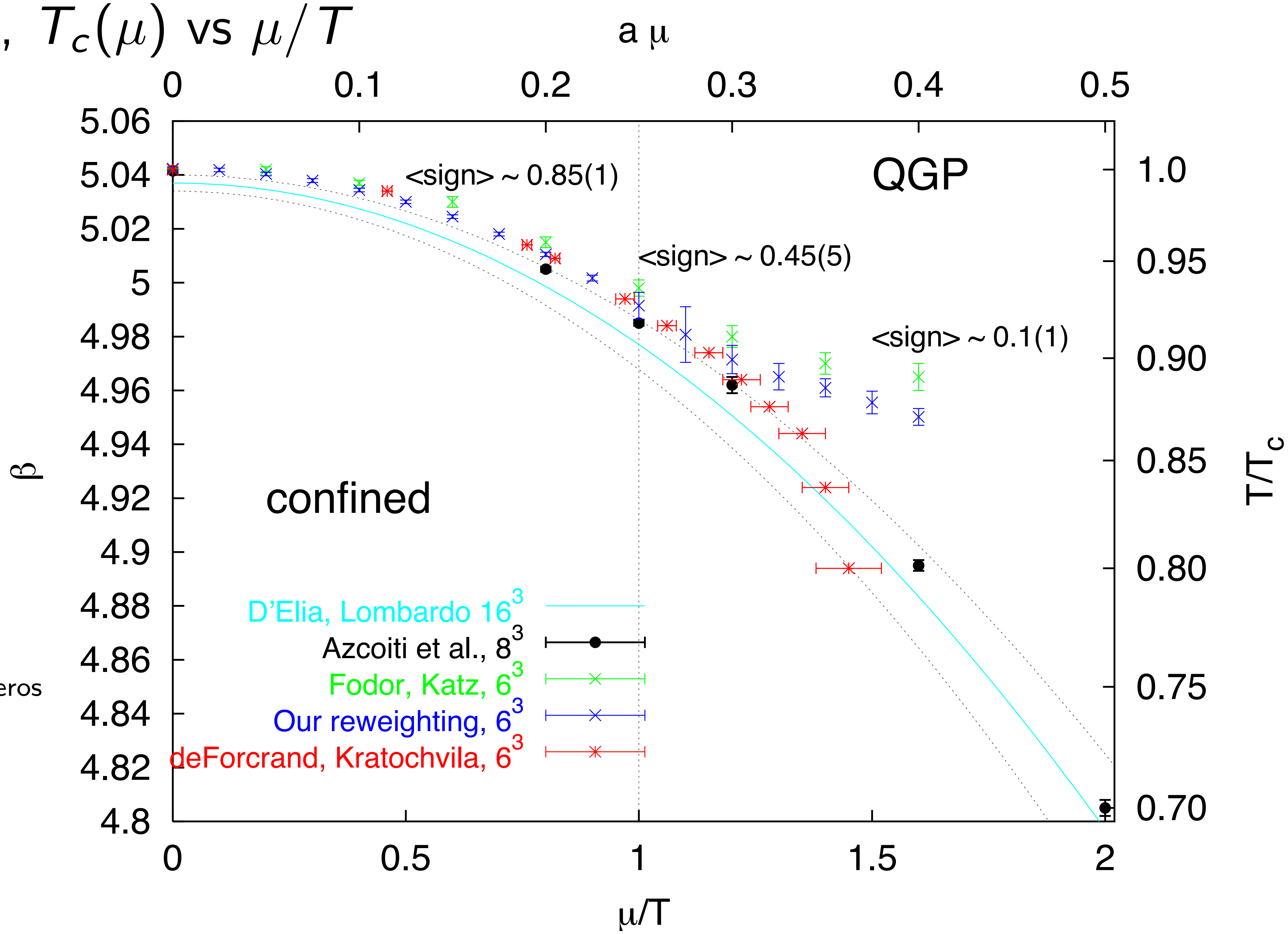
$$\sigma(C) = \underbrace{\operatorname{sign}\left(\prod_{i=1}^{\#C} 2\,\mathrm{Re}(W(C_i))\right)}_{\sigma_B(C)} \times \sigma_F(C)$$



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

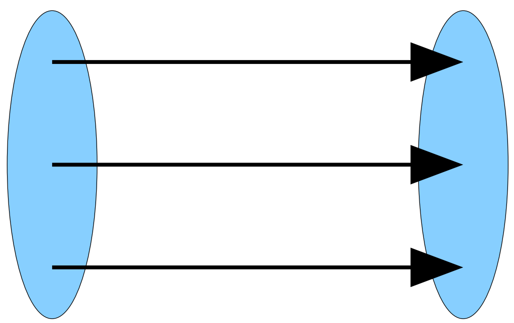
$N_f = 4$ staggered,
$am_q = 0.05$, $N_t = 4$
PdF & Kratochvila
LAT05

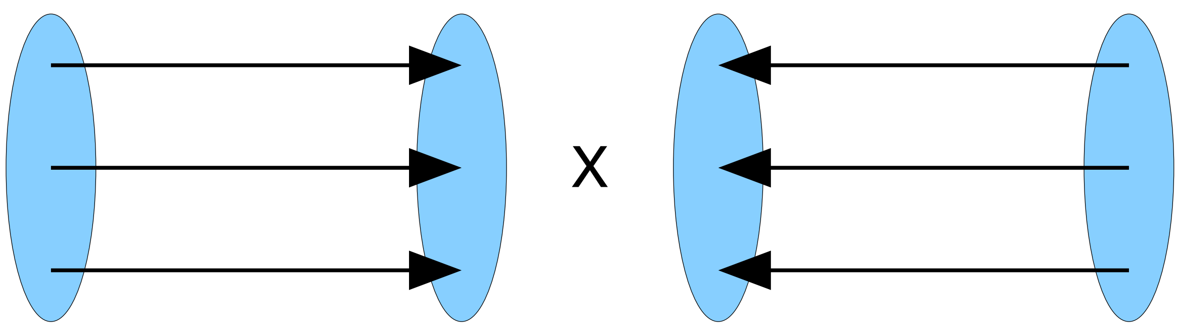
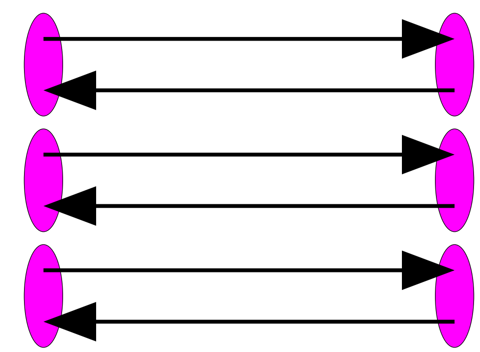
- Main results: - curvature of pseudocritical line $\frac{d^2 T_c}{d\mu^2}\Big|_{\mu=0}$
  - absence of critical point for $\frac{\mu}{T} \lesssim 1$

Alternative at $T \approx 0$: $\mu = 0$ + baryonic sources/sinks

Signal-to-noise ratio of N-baryon correlator $\propto \exp(-N(m_B - \frac{3}{2} m_\pi)t)$

Lepage 1989

$C_B(t) =$  $\sim \mathbf{e^{-m_B t}}$

$|C_B(t)|^2 =$  $\sim$  $\sim \mathbf{e^{-3 m_\pi t}}$

- Mitigated with variational baryon ops. $\rightarrow$ m_{eff} plateau for 3 or 4 baryons ?

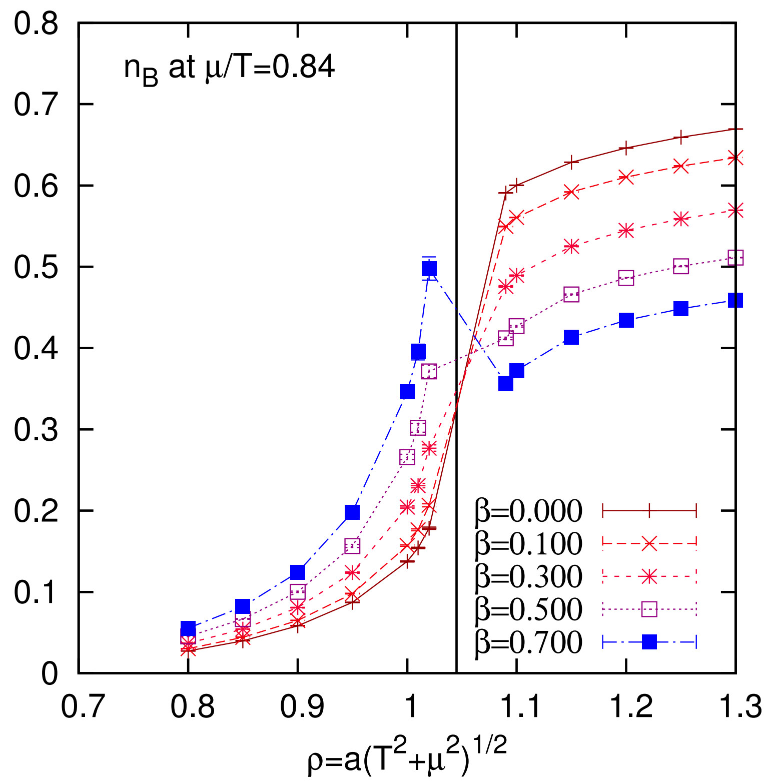
  Savage et al., 1004.2935

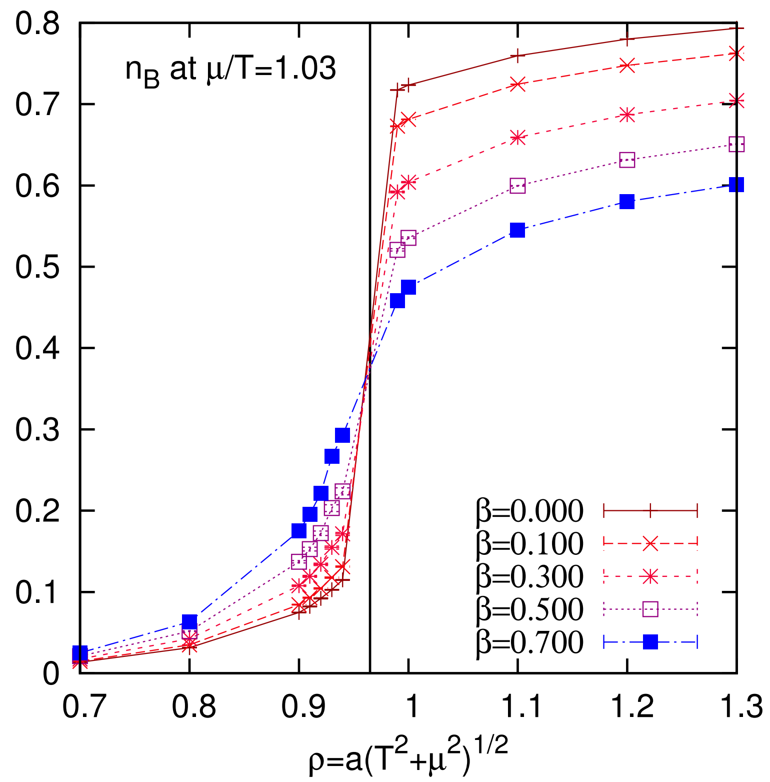
  At least 2 baryons $\rightarrow$ nuclear potential   Aoki, Hatsuda et al., eg. 1007.3559

- Beautiful results with up to 12$\rightarrow$72 *pions or kaons*   Detmold et al., eg. 0803.2728

  (cf. isospin-μ: no sign pb.)

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)

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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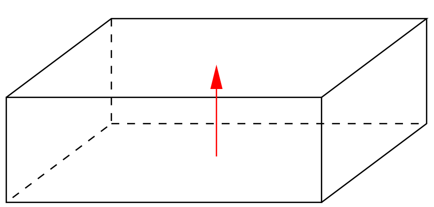
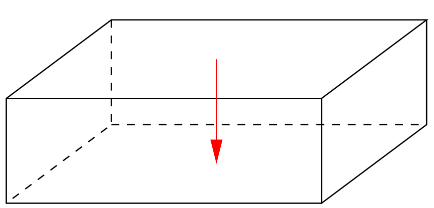


$$\langle \mathrm{Tr\ Polyakov} \rangle = \exp(-\tfrac{1}{T}F_{\mathbf{q}}) = \int \mathrm{Re\ Pol} \times \mathrm{Re}\ d\varpi - \mathrm{Im\ Pol} \times \mathrm{Im}\ d\varpi$$



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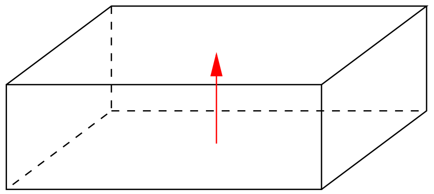

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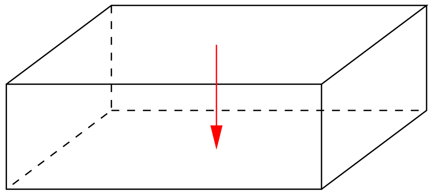

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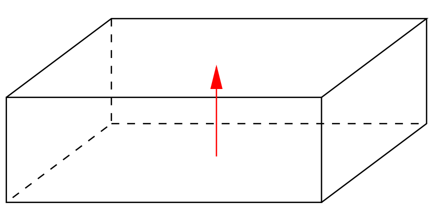

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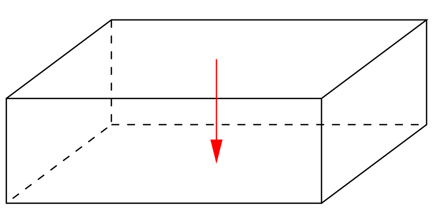

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Complex determinant $\Longrightarrow$ no probabilistic interpretation $\longrightarrow$ Monte Carlo ??

Sampling 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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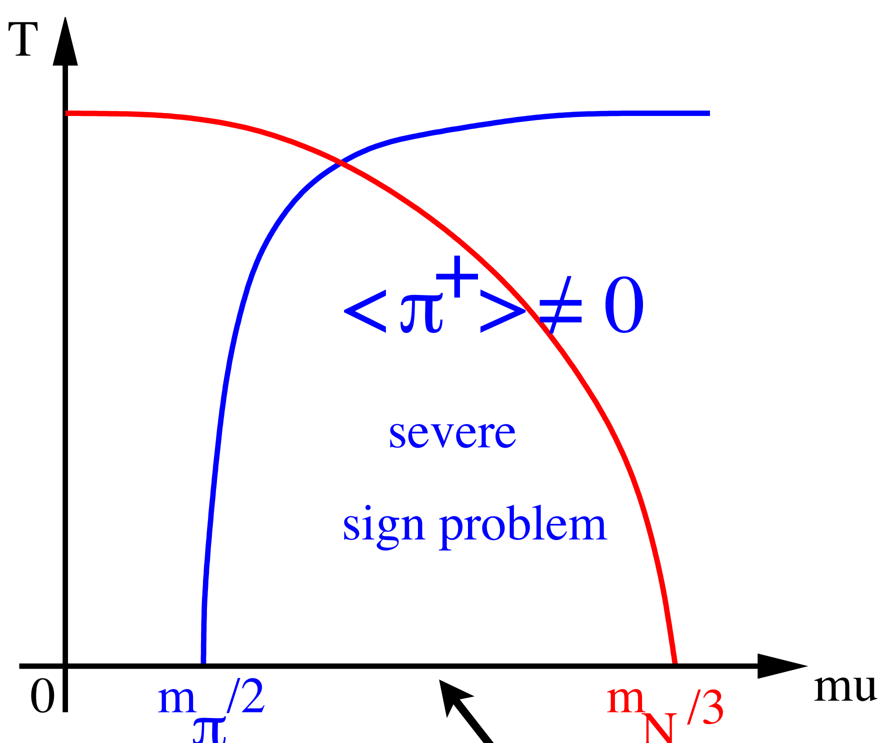

$\Delta f(\mu^2, T)$ large in the Bose phase
$\rightarrow$ "severe" sign pb.

"Silverblaze pb": phase of det changes groundstate

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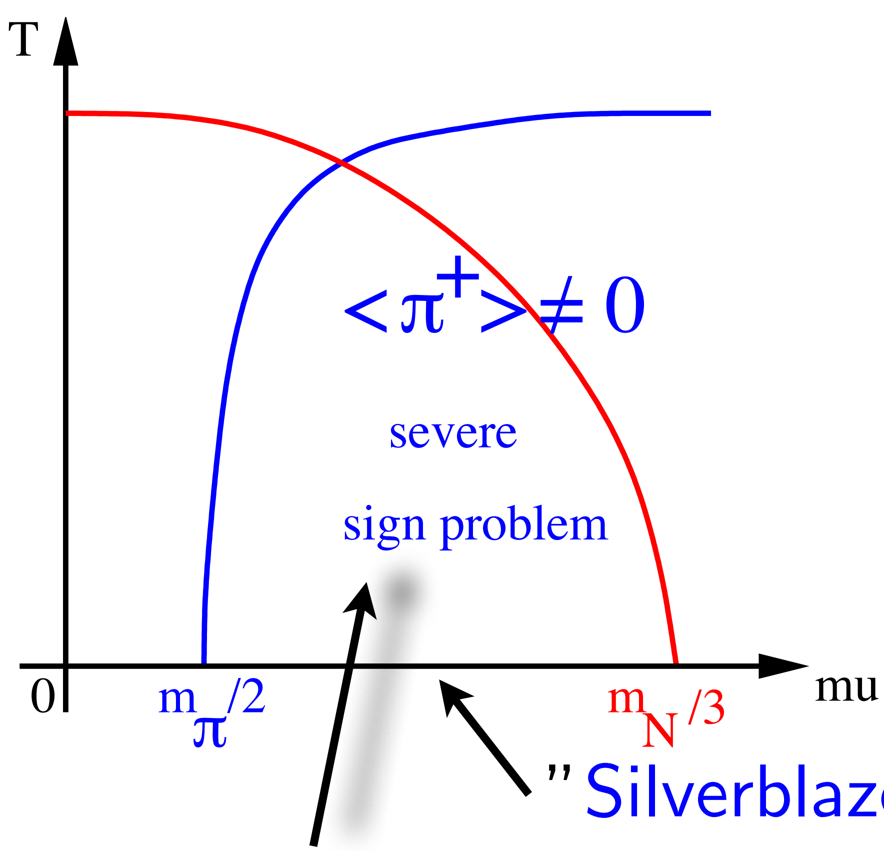

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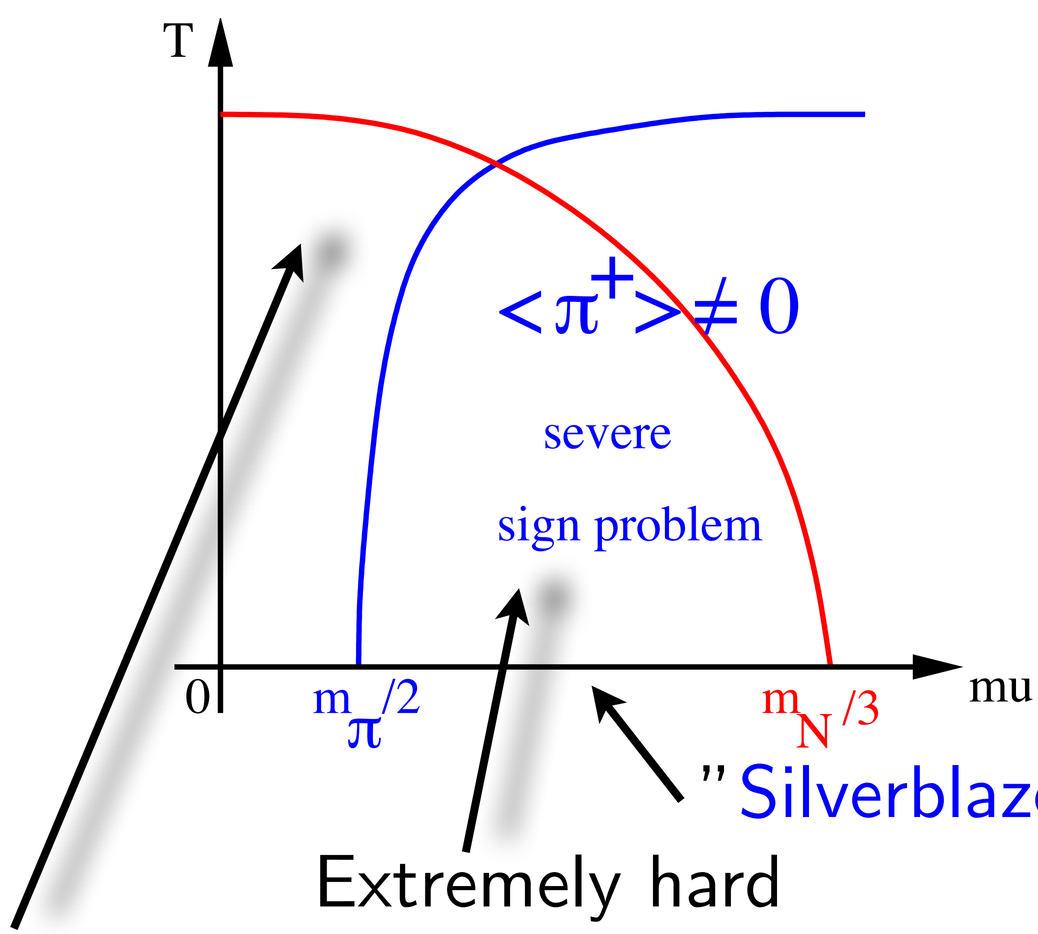

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Not as hard
$\frac{\mu}{T} \lesssim 1$