QCD at finite density on the lattice

Philippe de Forcrand
ETH Zürich & CERN

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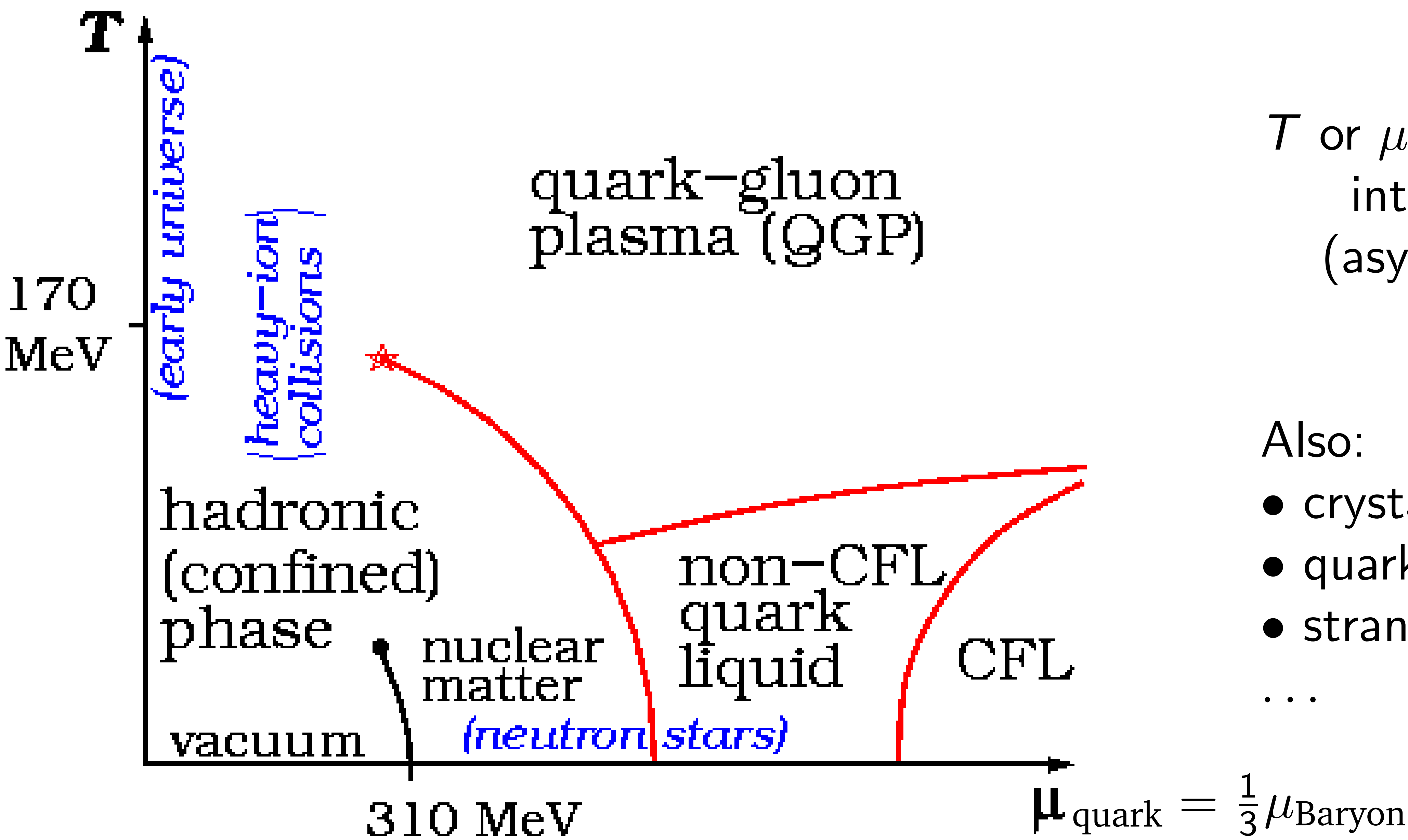
ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Motivation

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

phase transitions $\rightarrow$ non-perturbative $\rightarrow$ Lattice QCD

The wonderland phase diagram of QCD from Wikipedia



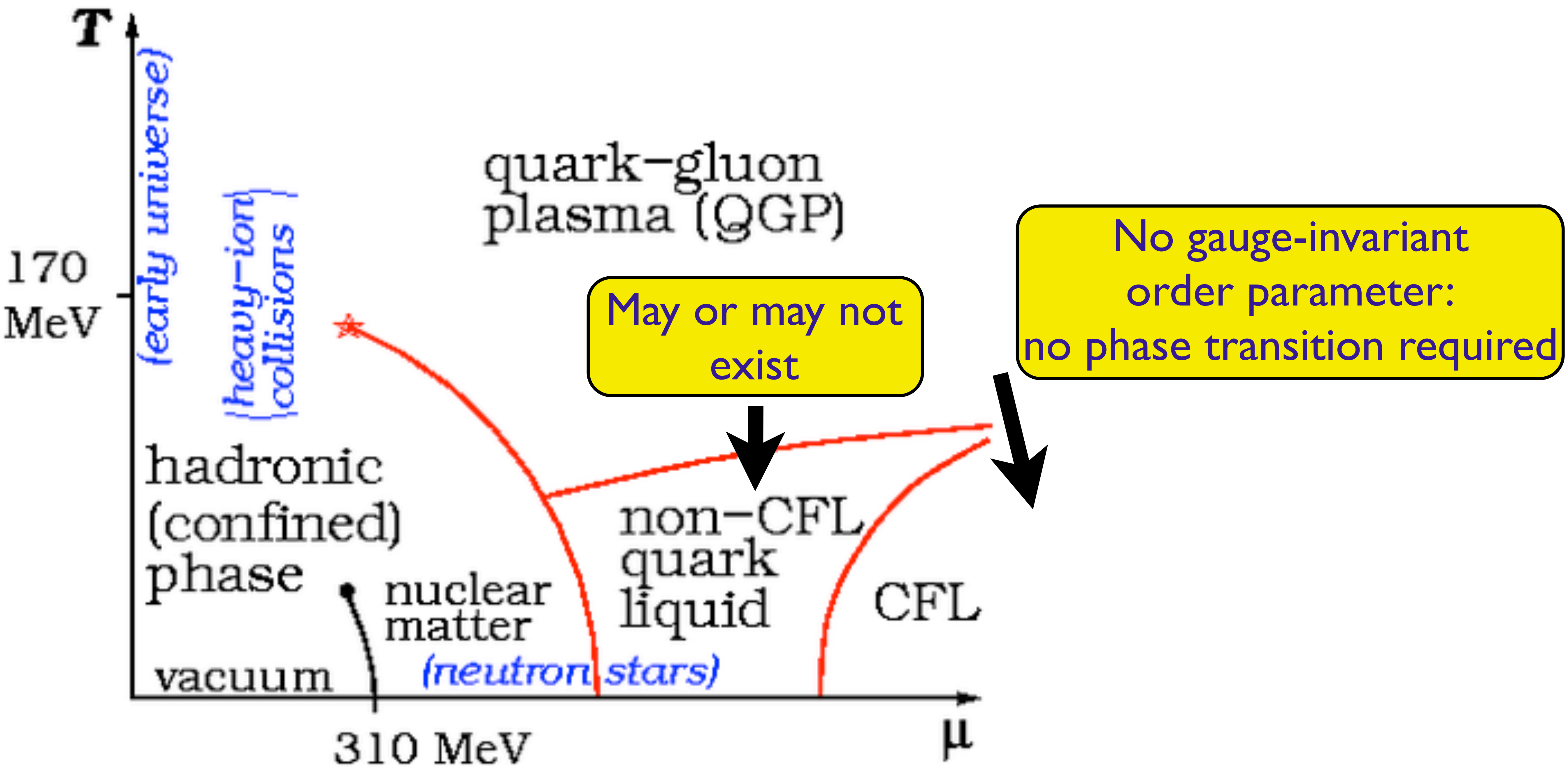
T or $\mu \to \infty$:
interaction weak
(asymptotic freedom)

Also:

- crystal phase(s)
- quarkyonic phase
- strangelets

...

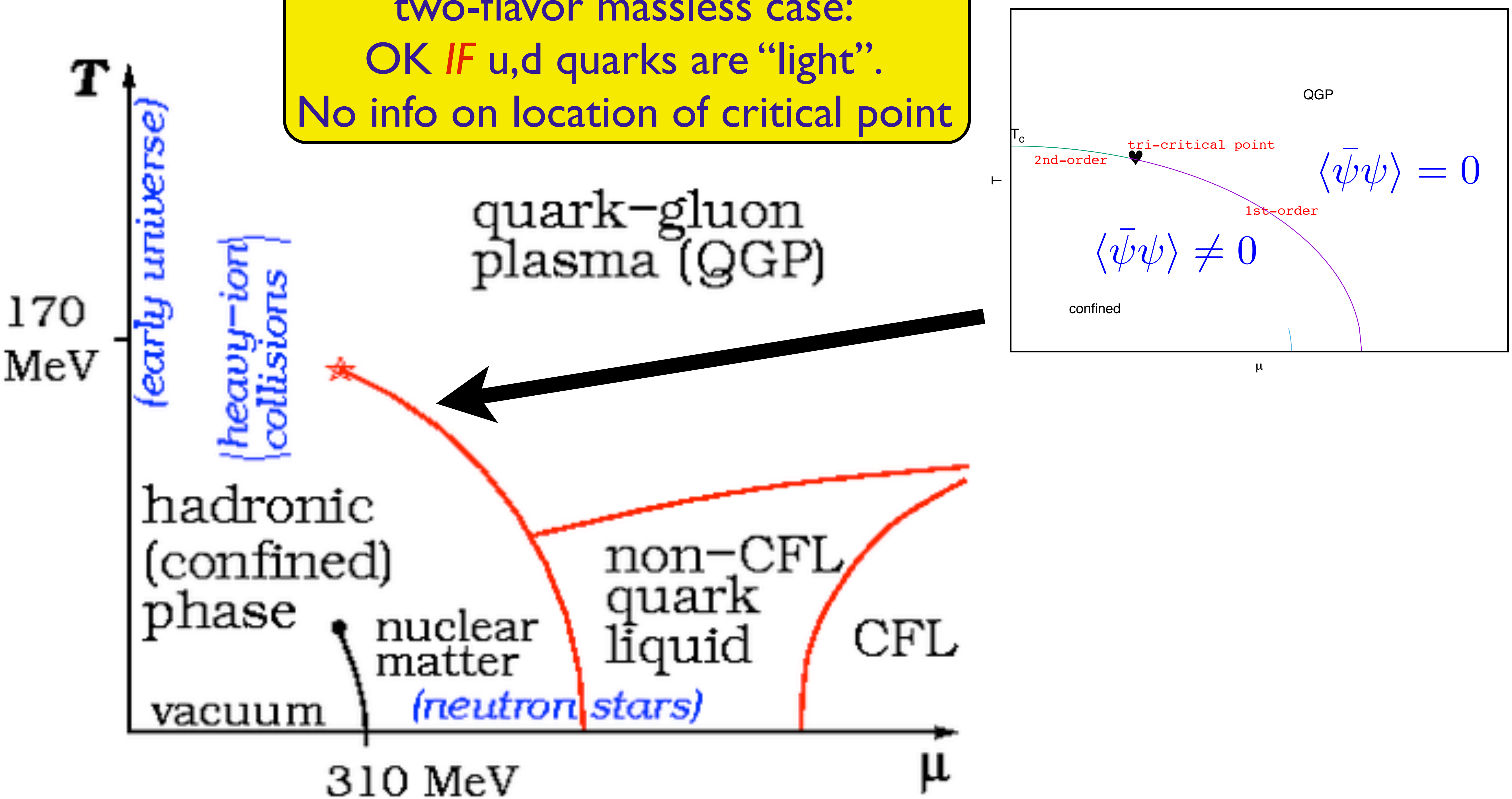
Caveat: everything in red is a conjecture



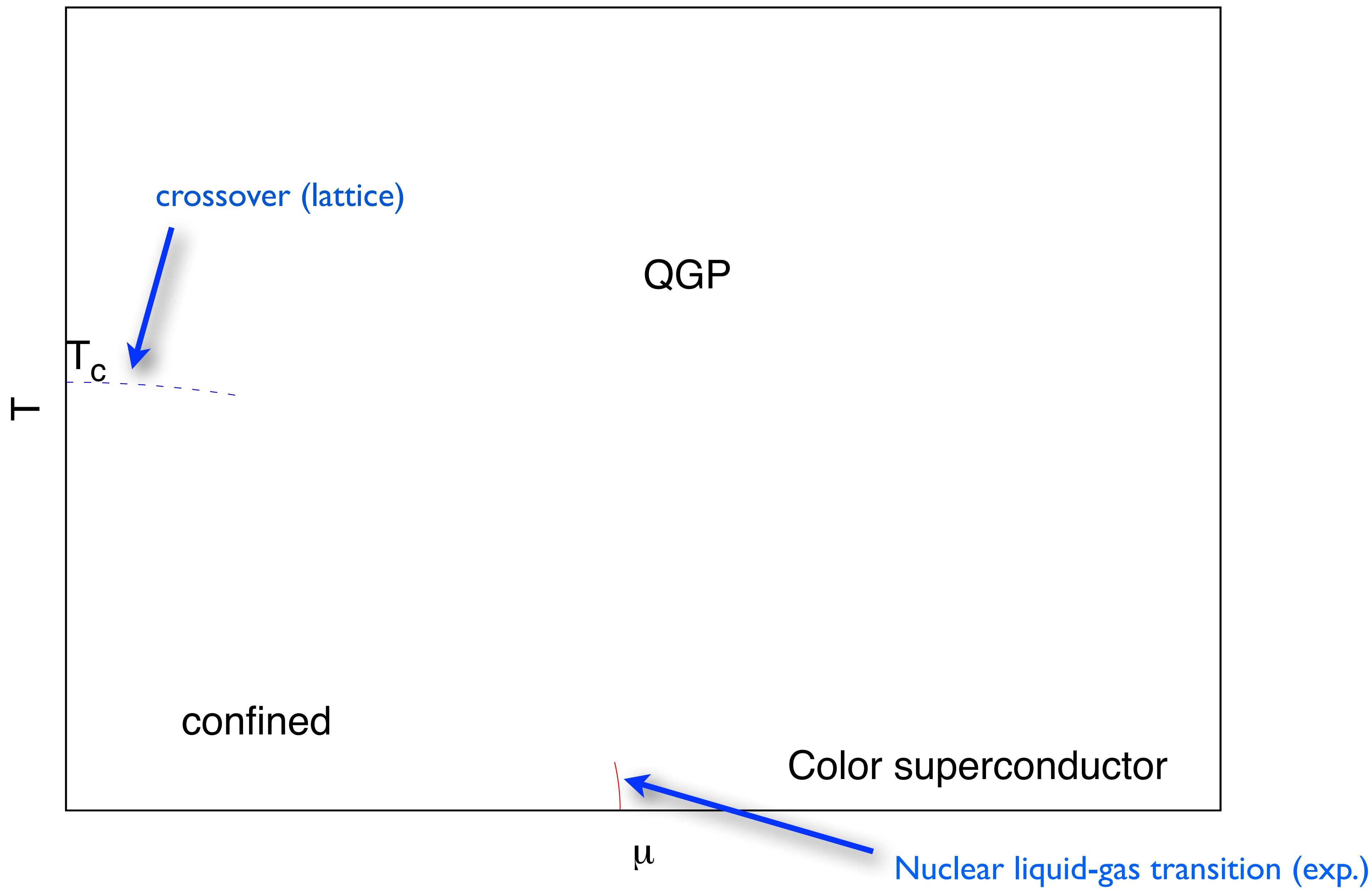
T
170
MeV
(early universe)
(heavy-ion)
(collisions)
quark−gluon
plasma (QGP)
May or may not
exist
No gauge-invariant
order parameter:
no phase transition required
hadronic
(confined)
phase
nuclear
matter
non−CFL
quark
liquid
CFL
vacuum
(neutron stars)
310 MeV
μ

“Small” deformation of
two-flavor massless case:
OK *IF* u,d quarks are “light”.
No info on location of critical point

$N_f = 2, m_u = m_d = 0$



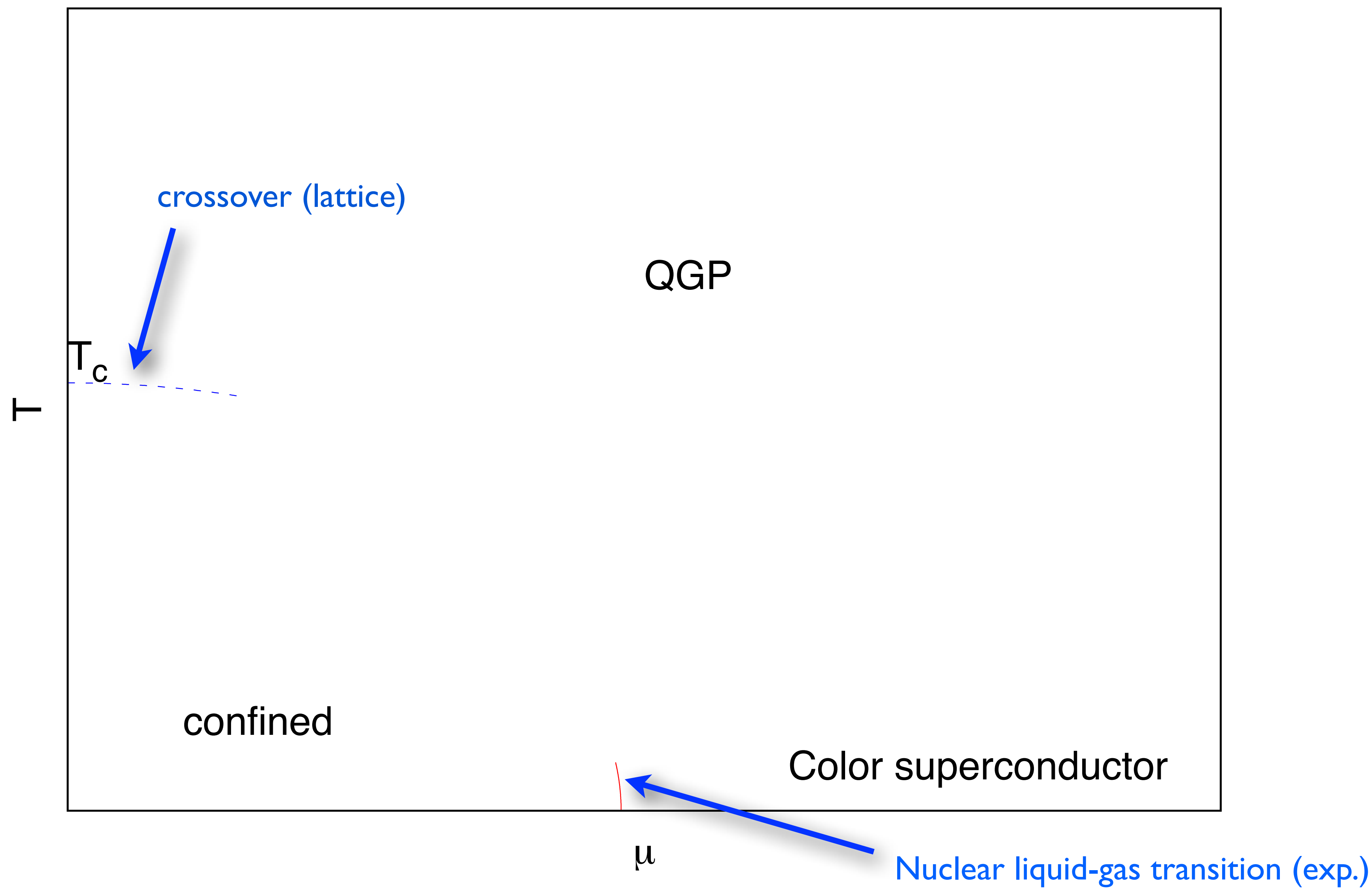
Finite μ: what is known?



Minimal, possible phase diagram

Finite μ: what is known?

Lattice: Sign problem *as soon as $\mu \neq 0$*



Minimal, possible phase diagram

"Sign problem" a.k.a. complex action pb: $\exp(-S) \notin \mathcal{R}_{\geq 0}$

Finite-density QCD: + Hubbard model, quantum time evolution, ...

Real > 0 "Boltzmann weight" is the exception rather than the rule

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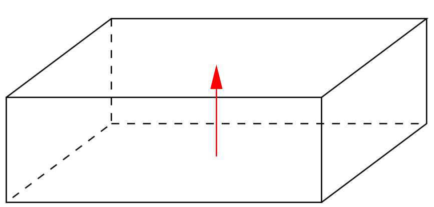
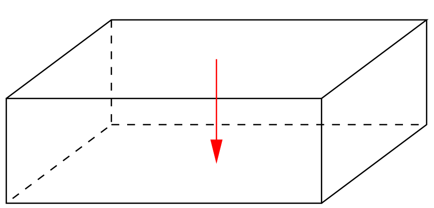
- Measure $d\varpi \sim \det \not{D}$ *must be complex* to get correct physics:



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



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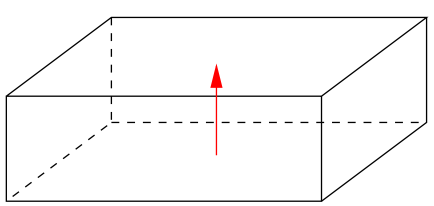

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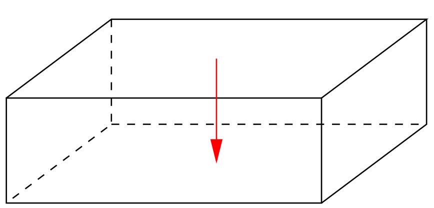

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- Origin: $\mu \neq 0$ breaks charge conj. symm., ie. usually complex conj.

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

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 $\approx \frac{1}{\sqrt{\#\ \ \mathrm{meas.}}}$

  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.

"Dual" variables

- Idea: strong-coupling/high-temperature expansion

$$\exp(\beta\ \phi_i^* \phi_j) \;=\; \sum_k \frac{\beta^k}{k!} \underbrace{(\phi_i^* \phi_j)^k}_{\text{integrate out}}$$

new Monte Carlo "dual" variable k for each link (ij)

- Partition function becomes gas of loops (particle worldlines)

- Loops have positive weights $\rightarrow$ sign problem gone! (not always)

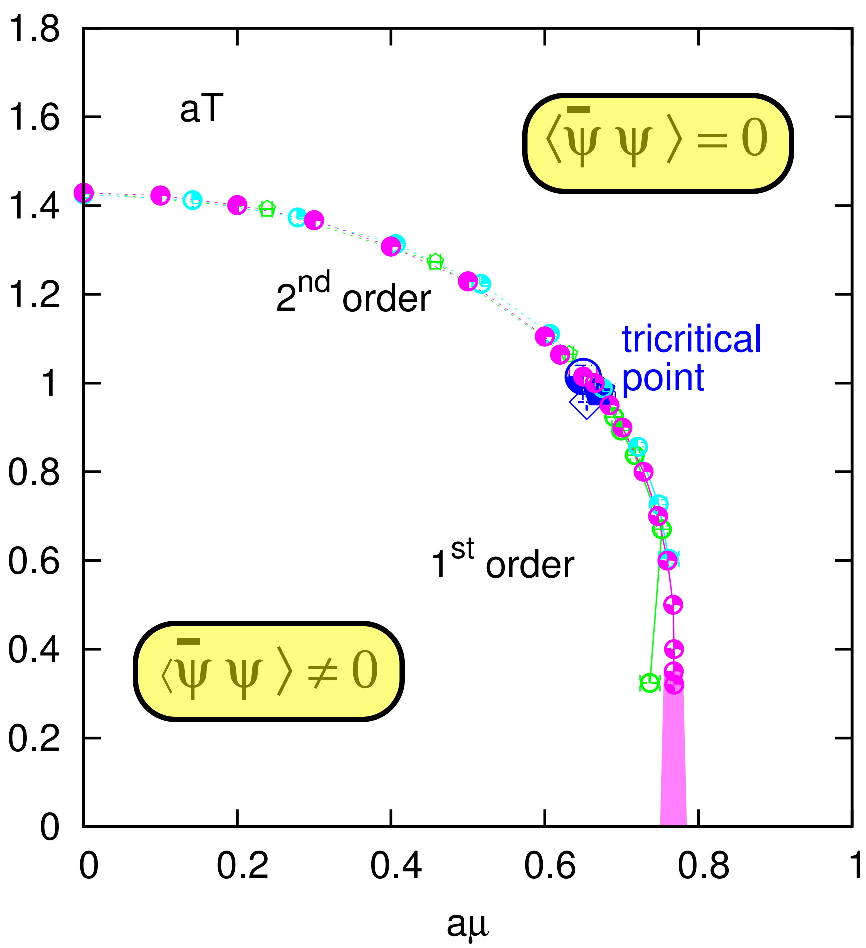
- Gauge fields: gas of surfaces; non-Abelian $\rightarrow$ sign problem again...

- QCD: ok for strong-coupling limit $\beta = \frac{6}{g^2} = 0$ (no plaquette term)

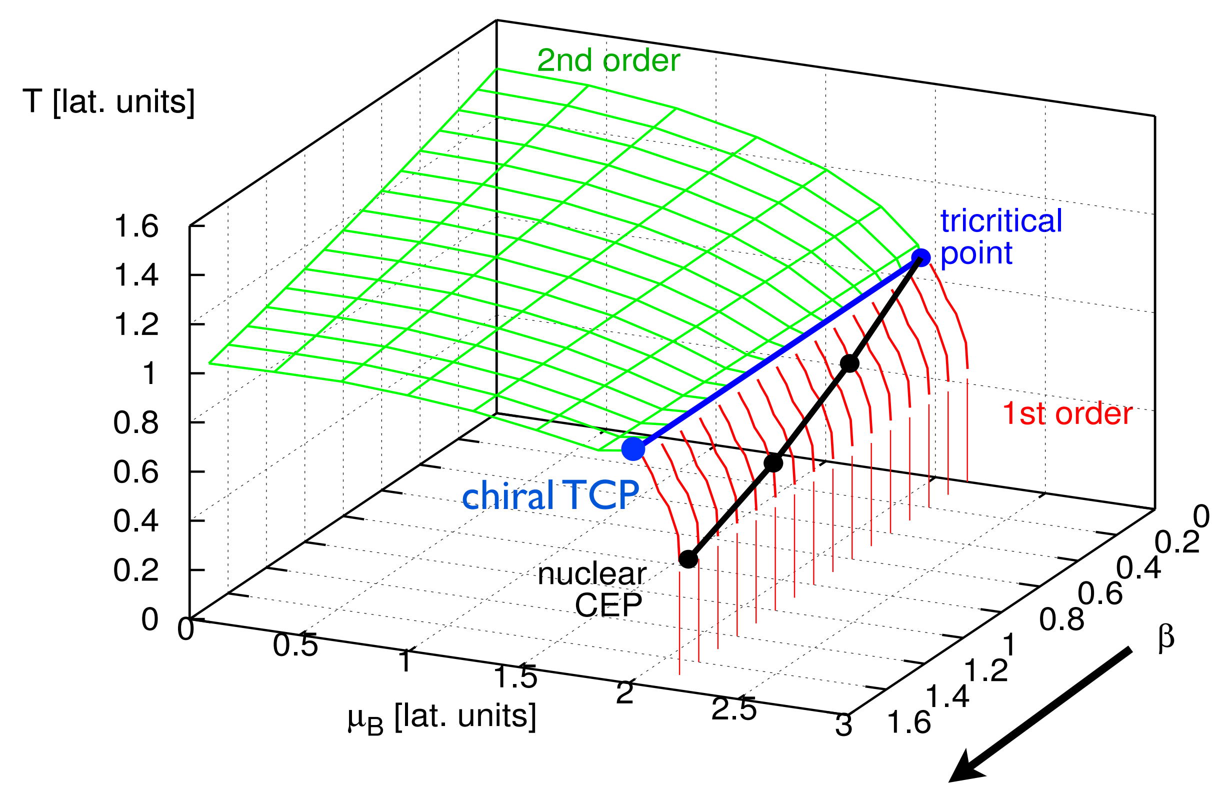
Results $\beta \approx 0$ w/Unger, Langelage, Philipsen

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

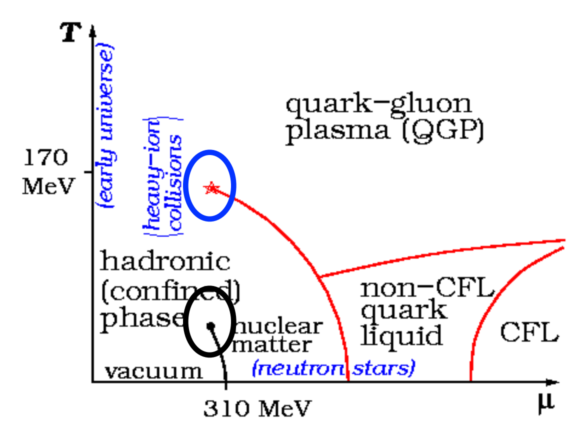
$\beta = 0$



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



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



Benchmark for other approaches

Methods under construction:

Field complexification

Witten

Going complex: difficulties with QCD

e.g. gauge field: $A_\mu \to A_\mu^R + iA_\mu^I$ $\quad S$ extended by analytic continuation

- QCD problem I:
  S is not analytic: $\log\det(\not{D})$ has poles and is multi-valued

- QCD problem II:
  gauge group $SU(3) \to SL(3,\mathcal{C})$, departure from $SU(3) \sim A_\mu^I$
  $SL(3,\mathcal{C})$ gauge transformations $\Rightarrow$ flat directions $A_\mu \to i\infty$
  $\Rightarrow$ runaway solutions; large, diverging force; roundoff error; etc..
  - gauge cooling — Seiler, Sexty & Stamatescu
  - irrelevant (?) $SU(3)$-restoring force — Attanasio & Jäger

Going complex I: doubling the number of d.o.f.

- Intelligent design: construct "representation" $P(A_\mu^R, A_\mu^I) \in \mathcal{R}^+$ such that

$$\langle W(A_\mu^R) \rangle_{\exp(-S_R - iS_I)} = \langle W(A_\mu^R + iA_\mu^I) \rangle_P \quad \forall W$$

Salcedo, Wosiek

Example: $S = (x - i)^2 \;\rightarrow\; P(x, y) = \delta(y - 1)\exp(-x^2)$

Finding suitable "representation" more difficult than solving the sign problem?

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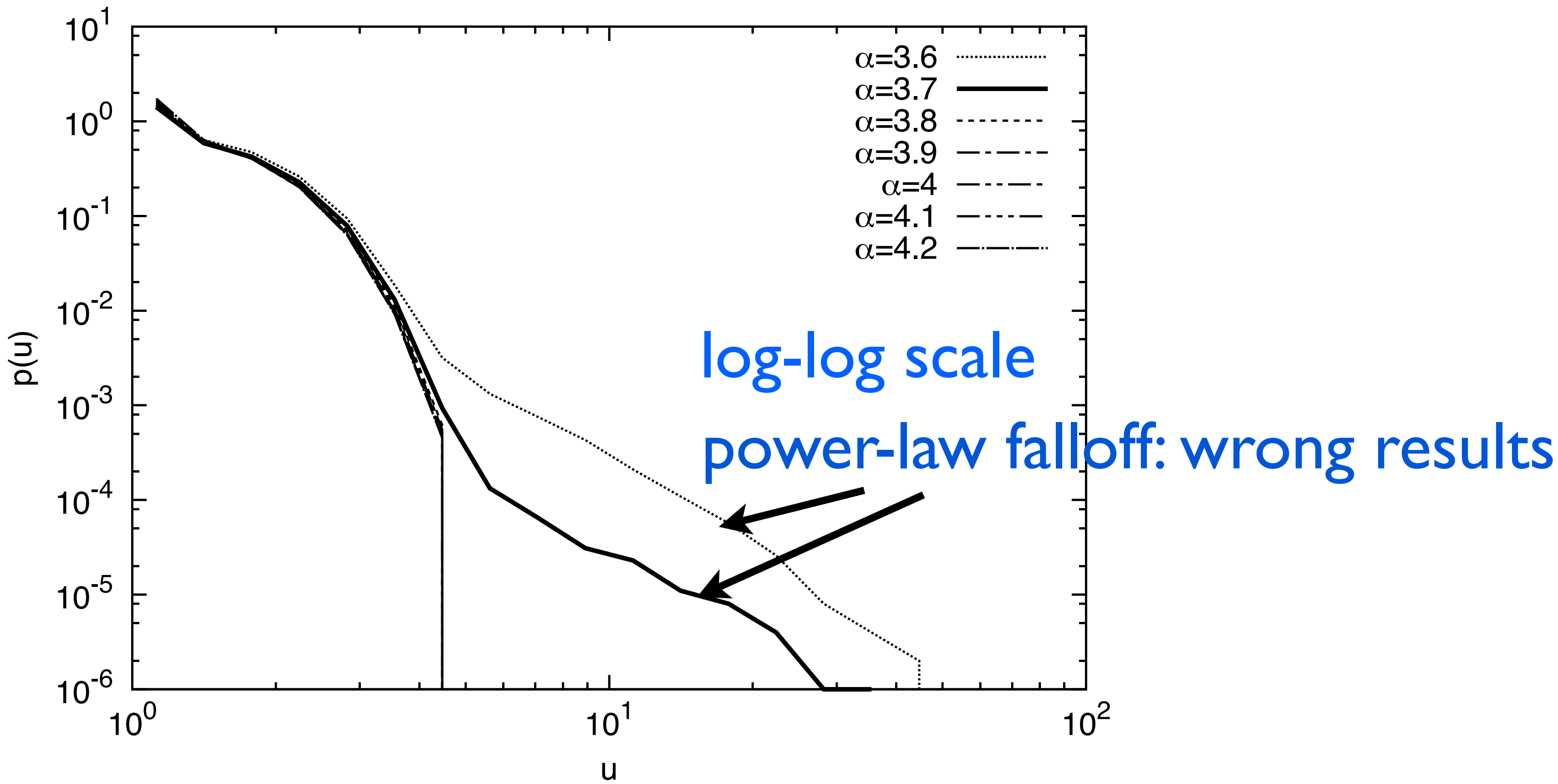
- Complex Langevin: *conjecture* by Parisi and by Klauder, 1983 $\frac{\partial \phi}{\partial \tau} = -\frac{\delta S}{\delta \phi} + \eta$
S complex $\rightarrow$ complex drift force ∇S, + complex noise
Outcomes: runaway, convergence to correct or to wrong answers
When does complex Langevin give correct results?
  - infinite set of conditions (Seiler et al) – not practical
  - no boundary in parameter space separating correct and wrong results
  $\rightarrow$ always wrong? Kogut & Sinclair?
  - real noise only
  - may give wrong answers in the absence of sign pb ($3d$ XY model, Aarts & James, 2010)

BUT

- Criterion for correctness (with proof): Nishimura et al, 1606.07627v4

  Distribution of drift force falls off *exponentially (or faster)*



- Modify this distribution (if necessary) by *extra drift force* and extrapolate results to zero such force Nishimura et al, Jaeger et al

- QCD with light quarks, low T large μ: under way! Nishimura et al Sexty et al, Kogut Sinclair

Going complex II: deforming the contour

- Lefschetz thimble:

Idea: deform integration contour in the complex plane,
such that $S_I = \text{constant} \to \approx$ constant phase

- do NOT explore full complexified space ($\leftrightarrow$ complex Langevin)
- to find the thimble: start at saddle point $\partial_z S(z) = 0$
  keep S_I fixed
  move to increase S_R (steepest ascent)
- IF one thimble, then constant phase e^{iS_I} cancels in vevs
  residual, mild sign pb from Jacobian along [not straight] thimble
  technical difficulty of sampling along thimble can be overcome

Di Renzo et al, Tanizaki et al, Fujii et al, Bedaque et al

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Problem: number of thimbles $\sim \exp(\text{Volume})$?

- Keep dominant thimble only (OK as $V \rightarrow \infty$?) but, eg. phase transitions??
- Keep all thimbles: - relative phase $\rightarrow$ sign pb reappears
  - ergodic sampling?

Going complex II: deforming the contour

- Holomorphic gradient flow: Alexandru, Bedaque et al, 1512.08764,..

Idea: tuning knob (flow time) to interpolate between real manifold and thimble

- $t = 0 \rightarrow$ original field ϕ
- $t > 0 \rightarrow \frac{d\phi}{dt} = \overline{\frac{\partial S}{\partial \phi}}$

Along flow, S_I remains constant, and S_R keeps increasing
ie. $\exp(-S_R)$ keeps decreasing, except for critical points $\partial S / \partial \phi = 0$
$\Longrightarrow$ approach Lefschetz thimbles as $t \rightarrow \infty$

Flow time:	0	$\longrightarrow$	∞
Difficulty:	sign pb		ergodicity pb
		sweet spot	

Note: sign pb requires $\exp(V)$ resources, ergodicity pb ALSO
$\rightarrow$ don't expect "sweet spot" to beat $\exp(V)$ complexity – only Δf smaller

- Path Optimization Method: minimize sign pb, using *Neural Network*

Ohnishi et al

Mature methods with limited scope:

Taylor expansion in μ/T

Small-μ approach: Taylor expansion

- Expansion parameter $\mu/T \lesssim 1$

$$P(T,\mu) - P(T,0) = \sum_{k=1} c_{2k}(T) \left(\frac{\mu}{T}\right)^{2k}$$

$$c_{2k} = \langle \mathrm{Tr} \text{ (degree 2k polynomial in } \not{D}^{-1}, \frac{\partial \not{D}}{\partial \mu} \text{) } \rangle_{\mu=0}$$

Standard $\mu = 0$ simulation & *noise vectors* to estimate Trace

- Combinatorial complexity in k $\rightarrow$ c_8 out of reach

$c_4 : 2002$
$c_6 : 2005$

- Progress: μ on the lattice
  - Linear: $U_4 \rightarrow (1 + a\mu)U_4$, UV divergence
  - 1983 Hasenfratz & Karsch: $U_4 \rightarrow \exp(a\mu)U_4$, cures UV divergence
  - 2011 Gavai & Sharma: linear + subtract UV divergence by hand ??

Taylor expansion: nitty-gritty

$$
\begin{aligned}
\frac{\partial^6 \ln \det M}{\partial \mu^6} &= \mathrm{tr}\left(M^{-1}\frac{\partial^6 M}{\partial \mu^6}\right) - 6\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial \mu}M^{-1}\frac{\partial^5 M}{\partial \mu^5}\right) \\
&-15\mathrm{tr}\left(M^{-1}\frac{\partial^2 M}{\partial \mu^2}M^{-1}\frac{\partial^4 M}{\partial \mu^4}\right) - 10\mathrm{tr}\left(M^{-1}\frac{\partial^3 M}{\partial \mu^3}M^{-1}\frac{\partial^3 M}{\partial \mu^3}\right) \\
&+30\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial \mu}M^{-1}\frac{\partial M}{\partial \mu}M^{-1}\frac{\partial^4 M}{\partial \mu^4}\right) + 60\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial \mu}M^{-1}\frac{\partial^2 M}{\partial \mu^2}M^{-1}\frac{\partial^3 M}{\partial \mu^3}\right) \\
&+60\mathrm{tr}\left(M^{-1}\frac{\partial^2 M}{\partial \mu^2}M^{-1}\frac{\partial M}{\partial \mu}M^{-1}\frac{\partial^3 M}{\partial \mu^3}\right) + 30\mathrm{tr}\left(M^{-1}\frac{\partial^2 M}{\partial \mu^2}M^{-1}\frac{\partial^2 M}{\partial \mu^2}M^{-1}\frac{\partial^2 M}{\partial \mu^2}\right) \\
&-120\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial \mu}M^{-1}\frac{\partial M}{\partial \mu}M^{-1}\frac{\partial M}{\partial \mu}M^{-1}\frac{\partial^3 M}{\partial \mu^3}\right) \\
&-180\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial \mu}M^{-1}\frac{\partial M}{\partial \mu}M^{-1}\frac{\partial^2 M}{\partial \mu^2}M^{-1}\frac{\partial^2 M}{\partial \mu^2}\right) \\
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\end{aligned}
$$

Now estimate all Traces by sandwiching between noise vectors... GPUs

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\end{aligned}
$$

Only term surviving with linear μ

Fewer traces $\rightarrow$ less work and more precise estimates

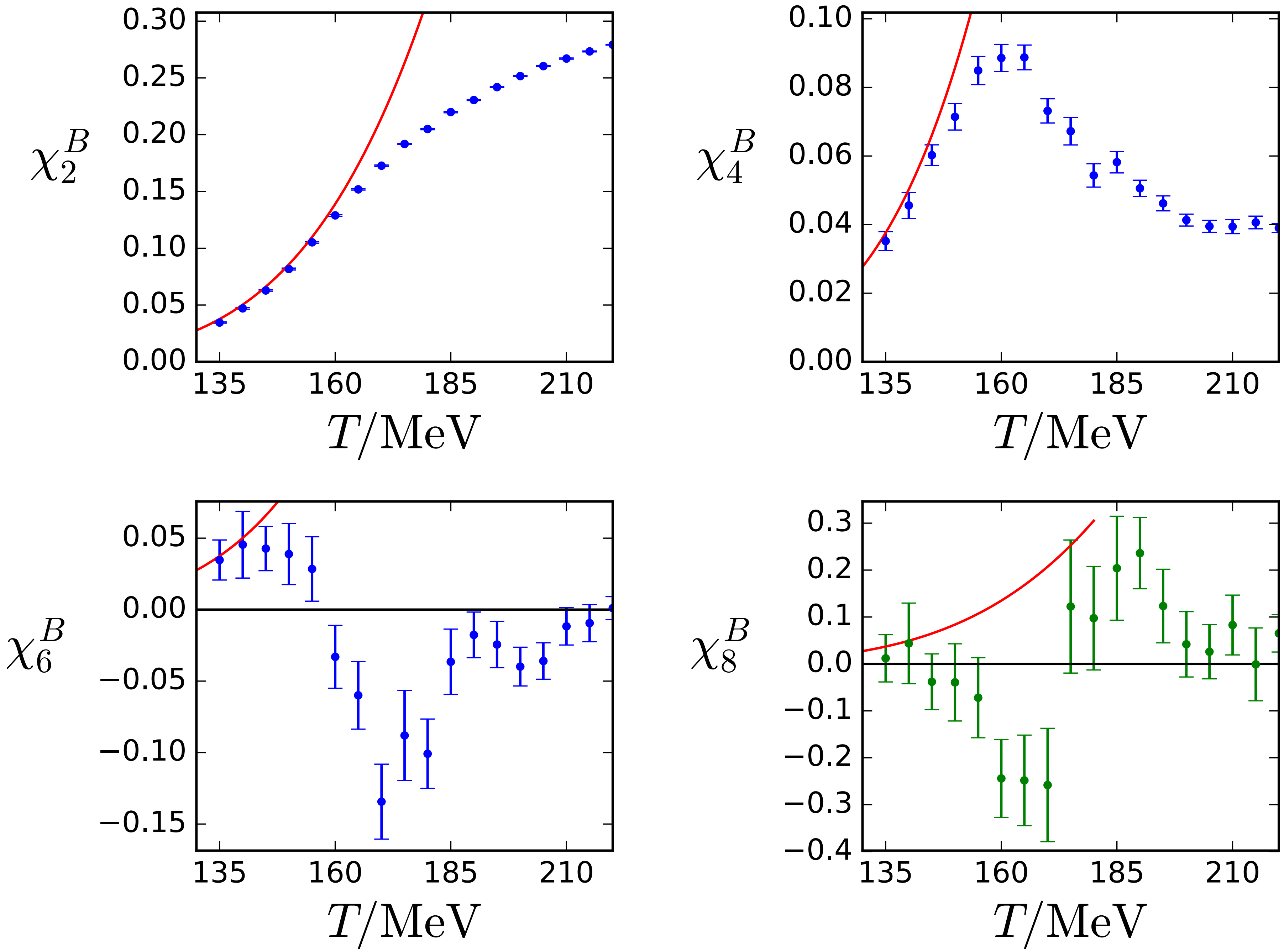
Small-μ approach: imaginary-μ

- Simulate at several values of $\mu = i\mu_I$: no sign pb.
  ($|\mu_I| < \frac{\pi T}{3}$, Roberge-Weiss singularity)
- Fit $\langle \mathcal{O} \rangle(\mu_I) = \sum_k \frac{d_k}{k!} \mu_I^k \quad \rightarrow \quad d_k$ is estimator of $\frac{\partial^k \mathcal{O}}{\partial \mu_I^k}$
  Analytic continuation trivial: $i\mu_I \rightarrow \mu$
- For pressure, take eg. $\mathcal{O} = n_B = \frac{\partial P}{\partial \mu_B}$ and integrate fitted polynomial
- Degree of fitted polynomial, fit range $\rightarrow$ systematic error?

New (Wuppertal): global fit (at each T) with Bayesian prior

1805.04445, Fodor et al.

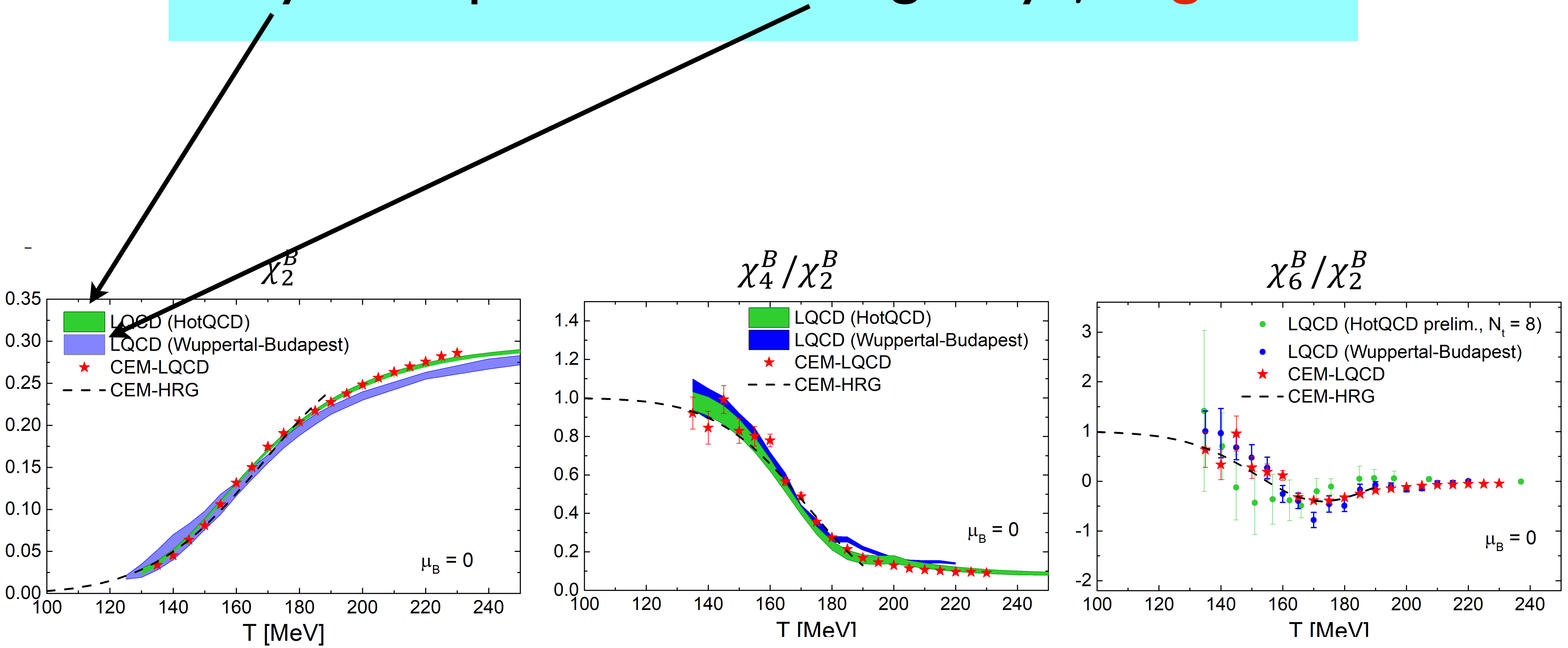
$N_\tau = 12$



c_8

Figure 2. Results for χ_2^B, χ_4^B, χ_6^B and an estimate for χ_8^B as functions of the temperature, obtained from the single-temperature analysis. We plot χ_8^B in green to point out that its determination is guided by a prior, which is linked to the χ_4^B observable by Eq. (3.4). The red curve in each panel corresponds to the Hadron Resonance Gas (HRG) model result.

Taylor expansion and imaginary-μ agree

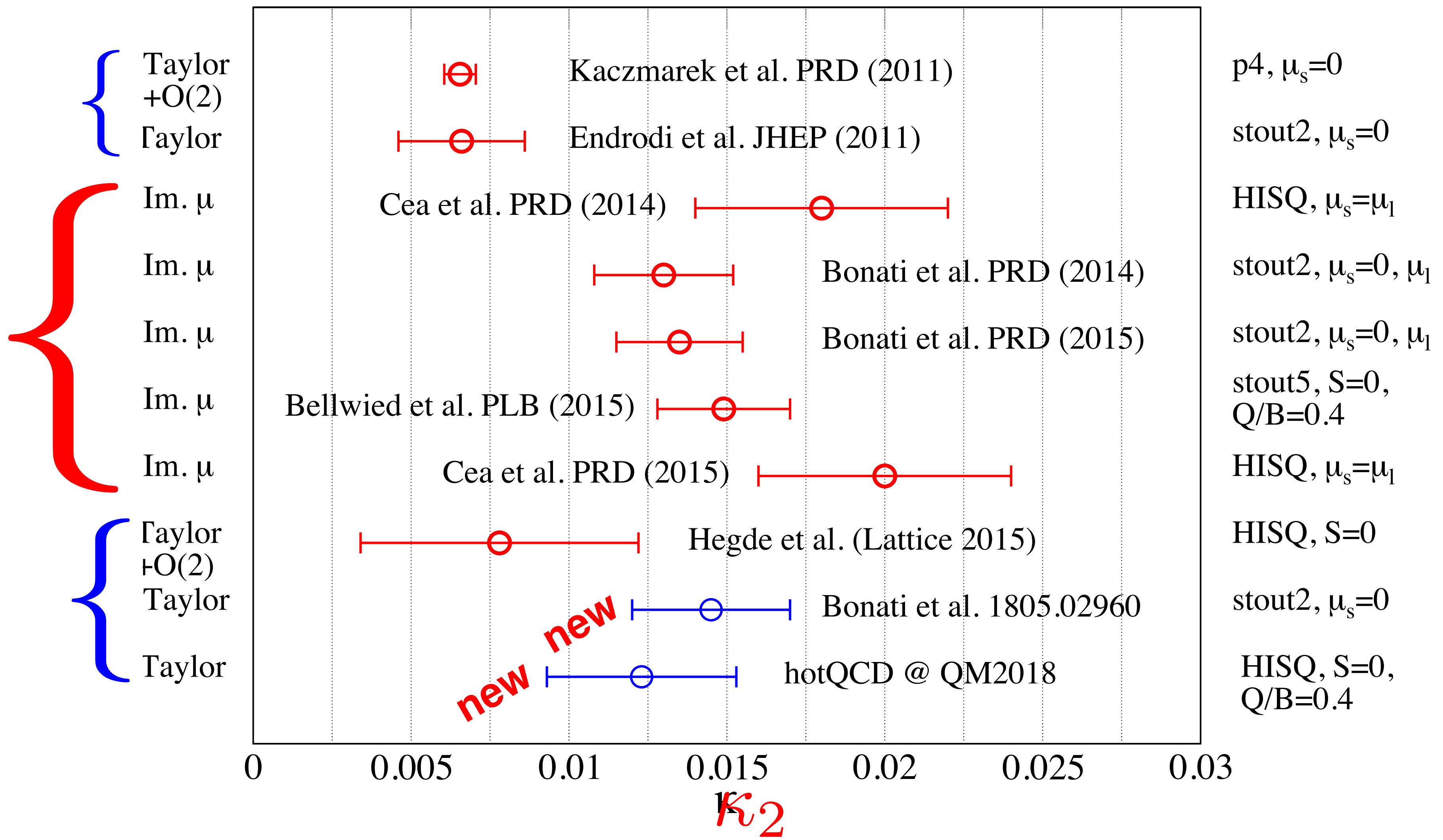


Vovchenko,
XQCD2018

Taylor expansion and imaginary-μ agree

Here, for curvature of pseudo-critical line:

$$\frac{T_c(\mu_B)}{T_c(0)} = 1 - \kappa_2 \left(\frac{\mu_B}{T_c(0)}\right)^2 + \mathcal{O}(\mu_B^4)$$



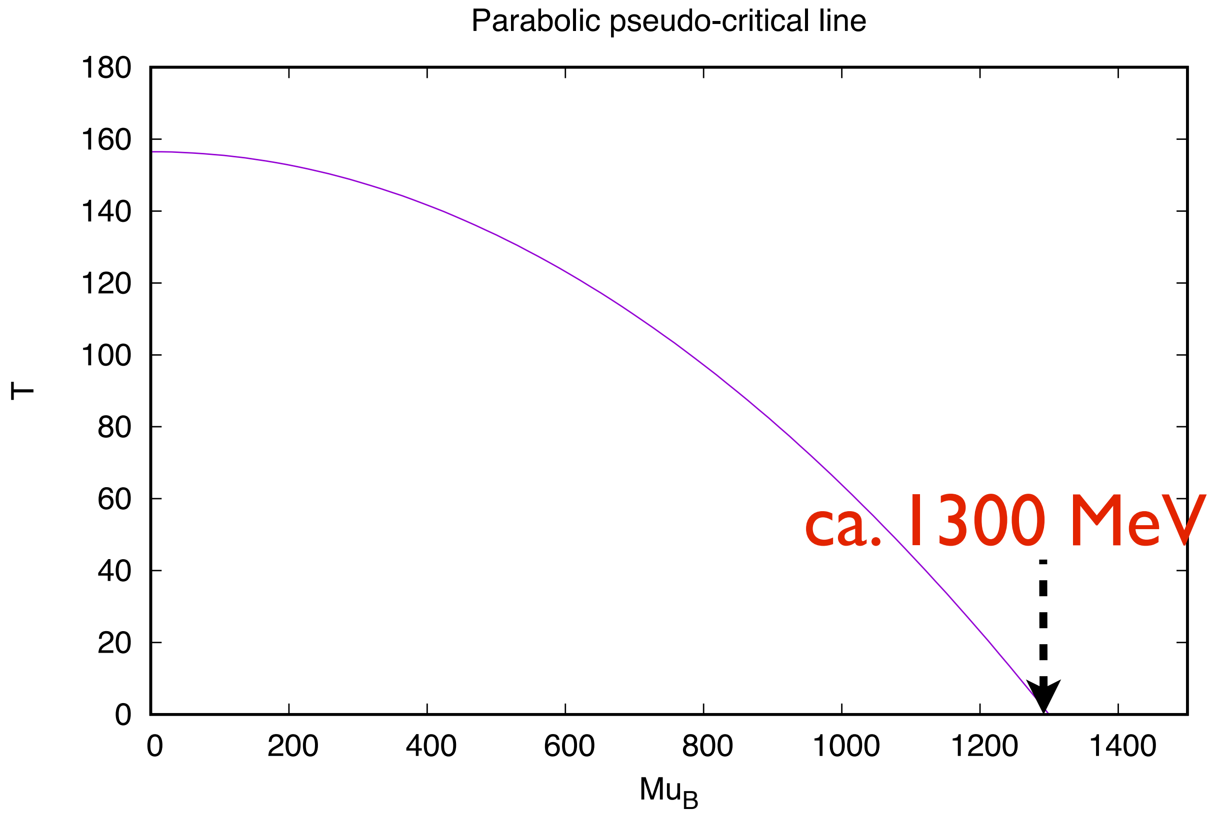
M. D'Elia, QM2018

Personal view

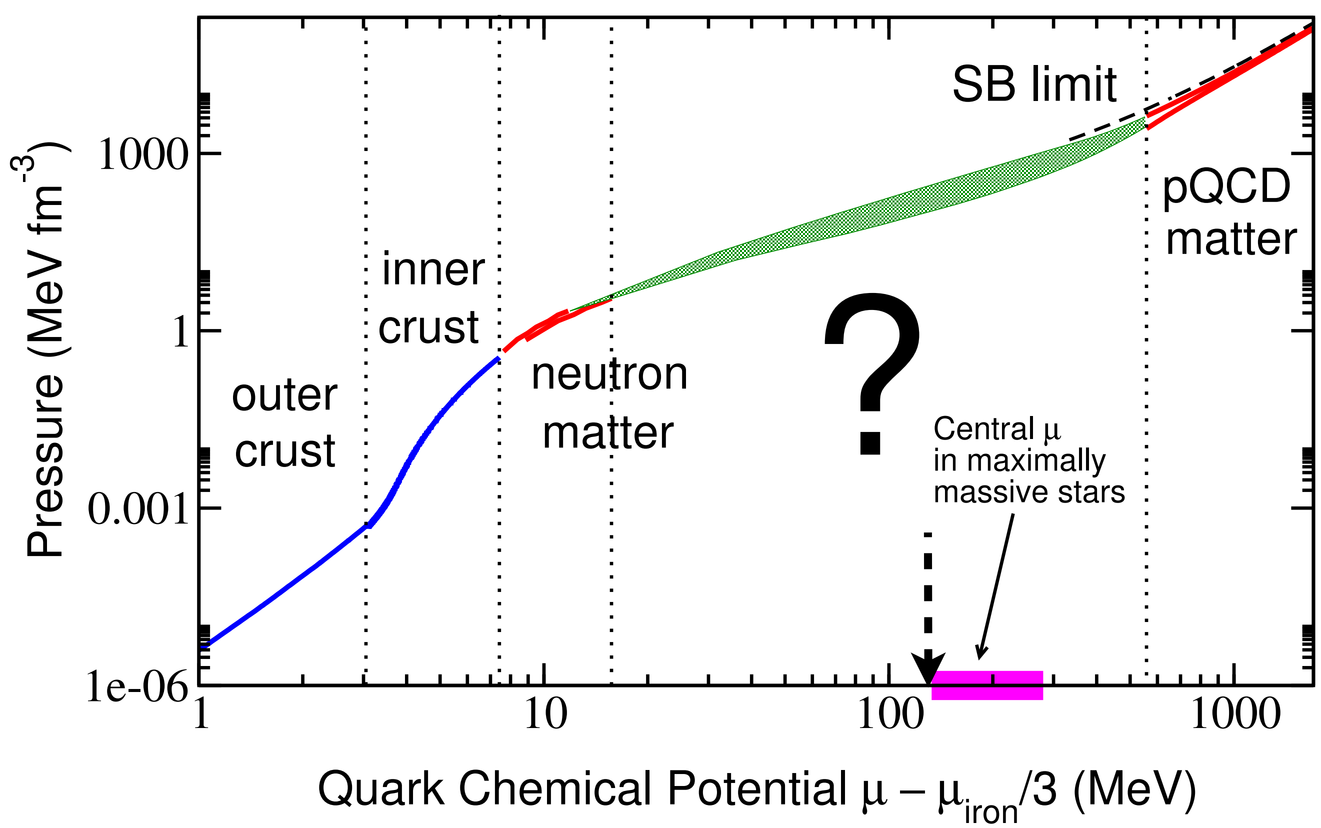
Prospects for a *relevant* QCD critical point are *receding*

- No signal [yet] from RHIC beam energy scan
- Large mass neutron stars disfavor quark matter core (EOS too soft)

- Curvature of pseudo-critical line is *small:*



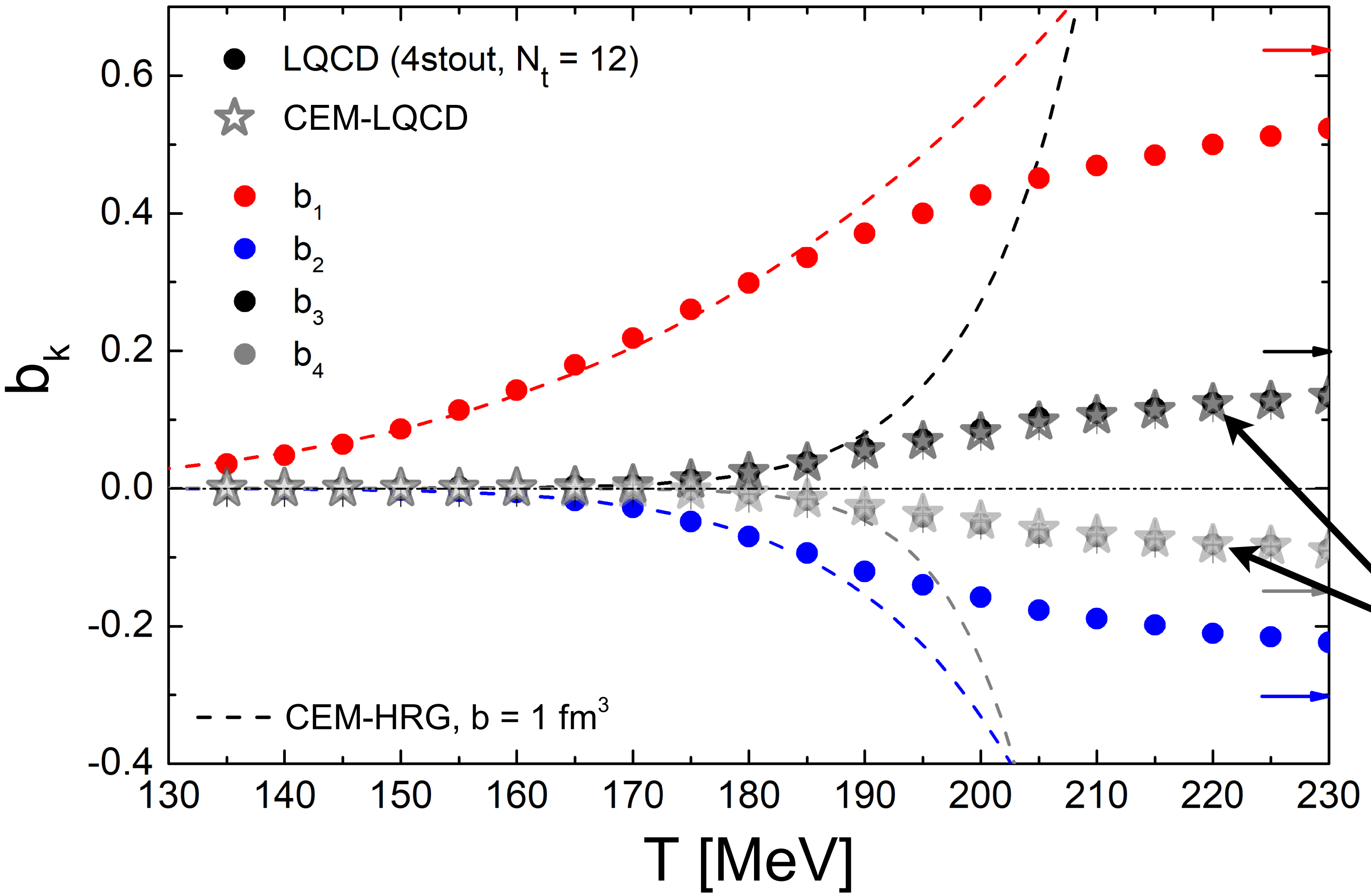
1402.6618, Kurkela et al.



- Models (PNJL, strong-coupling LQCD,..) place crit.pt. *far to the right*

Finding a crit.pt. at large μ requires **massive** CPU effort

or a breakthrough...



arXiv:1711.01261
Vovchenko et al.

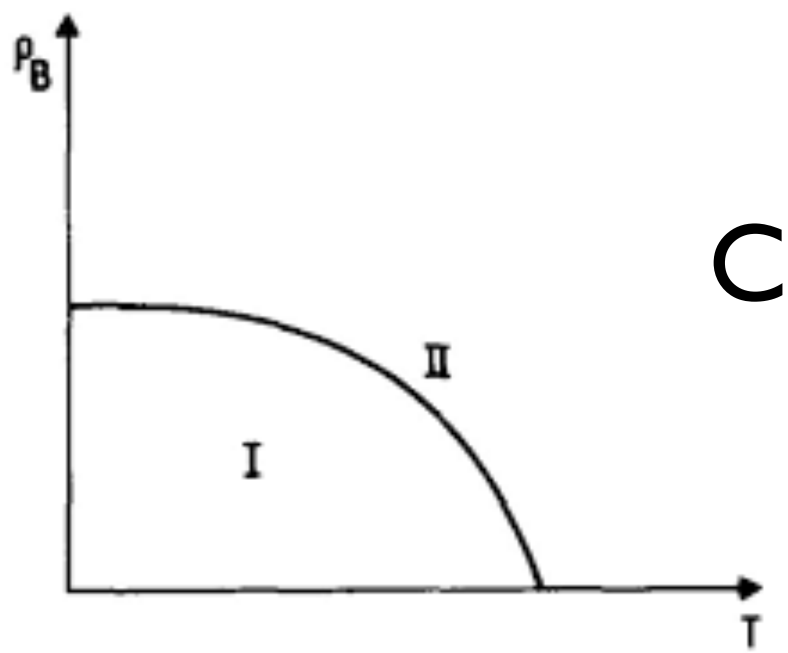
~ Taylor coeffs of pressure to 8th order versus T compared with Ansatz

stars & circles on top of each other

- At each temperature, Monte Carlo values of b_1, b_2 specify the Ansatz
- Then Ansatz predicts $b_3, b_4 \rightarrow$ perfectly consistent with Monte Carlo

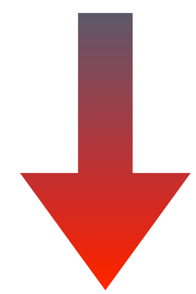
Analytic **Ansatz describes all available Monte Carlo data!**

Time evolution of the phase diagram of QCD



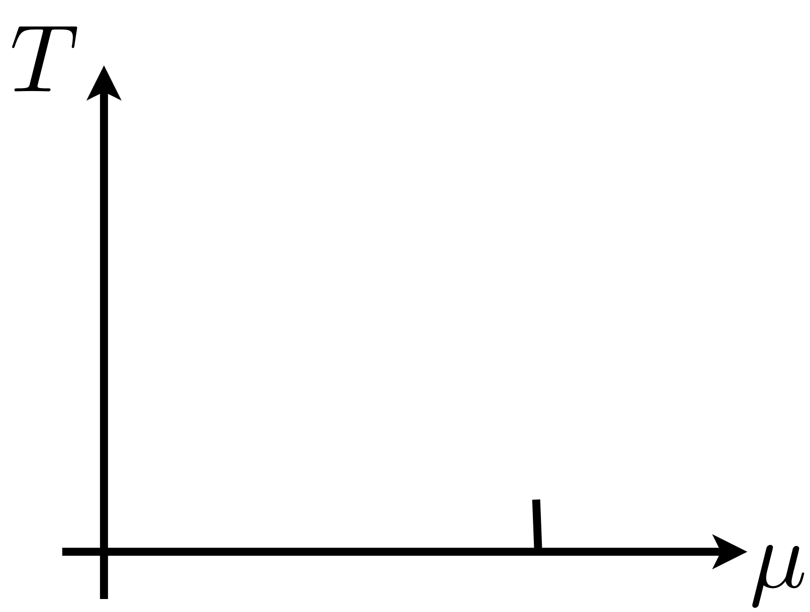
Cabibbo & Parisi, 1975

"little bang"

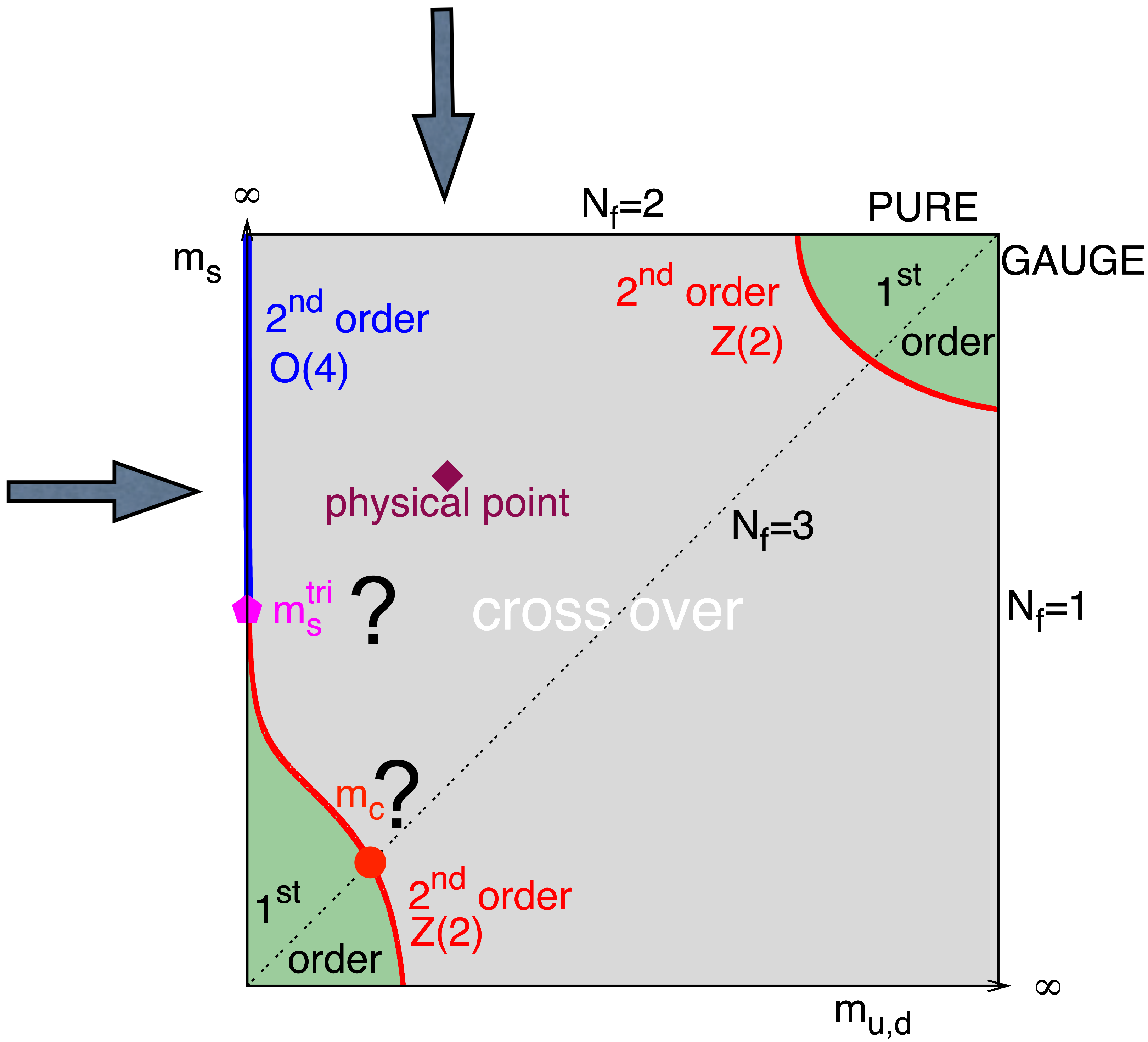


2020

"no bang at all" ?



Backup



∞
$N_f=2$
PURE
GAUGE
m_s
2^{nd} order
O(4)
2^{nd} order
Z(2)
1^{st}
order
physical point
$N_f=3$
m_s^{tri}
?
cross over
$N_f=1$
m_c
?
2^{nd} order
Z(2)
1^{st}
order
∞
$m_{u,d}$

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

- Strategy: choose $\{|\psi\rangle\}$ "close" to physical eigenstates of H

without full-fledged diagonalization of H

Strategy is general – "deep" optimization? tensor networks?

Catalogue of approaches to bypass the QCD sign pb

- Analytic continuation from imaginary μ (no sign pb there): data is cheap
  How to control systematic error?? (fitting ansatz)

- Taylor expansion in μ/T about $\mu = 0$:
  limited info $\mu/T \lesssim 1$
  cost of k^{th} coeff increases very steeply with k
  technical advances Gavai, Sharma, Schmidt,..

- Density of states:
  $S = S_R + iS_I$; select one observable eg. $S_I \to Z_x = \int \mathcal{D}U e^{-S_R} \delta(S_I - x)$
  $Z = \int dx\ Z_x\ e^{ix}$, i.e. Fourier transform
  old: Gocksch (1988), Fodor Katz & Schmidt, 2007, ..
  significant progress: Langfeld, Lucini & Rago, 2012
  Solves overlap pb
  consensus(?): data alone not accurate enough to beat sign pb:
  need "smoothing" or "fitting" ansatz LLR; Gattringer
  $\to$ bias PdF & Rindlisbacher, XQCD 2016

Catalogue of approaches to bypass the QCD sign pb: a sobering story (Ph.D. thesis, Slavo Kratochvila, ETH, 2005)

- Toy problem: estimate $\langle W(\lambda)\rangle = \frac{\int_{-\infty}^{+\infty} dx \;\; e^{-x^2+i\lambda x}}{\int dx \;\; e^{-x^2}}$

Exact answer: $\langle W(\lambda)\rangle = \langle e^{i\lambda x}\rangle_{\lambda=0} = e^{-\lambda^2/4} \rightarrow$ exponentially large cancellations

- One approach: deformation of contour in the complex plane

  Note saddle points: $x = i\lambda/2$ (numerator) and $x = 0$ (denominator)

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- One approach: deformation of contour in the complex plane

  Note saddle points: $x = i\lambda/2$ (numerator) and $x = 0$ (denominator)

- Observation: optimum is to go through $x = i\lambda/4$, ie. neither saddle point!

  Why? Moving the contour away from real axis renders denominator oscillatory

Sign problem is shifted between numerator and denominator!
Optimum contour is a compromise (half-way between the two saddle points)
which depends on observable W

Lesson for realistic problems:

an innocent observable may become oscillatory when analytically continued
$\rightarrow$ danger of simply reshuffling the sign pb from Z to W

cf. optimization of contour via cost-function   Ohnishi et al, 1705.05605

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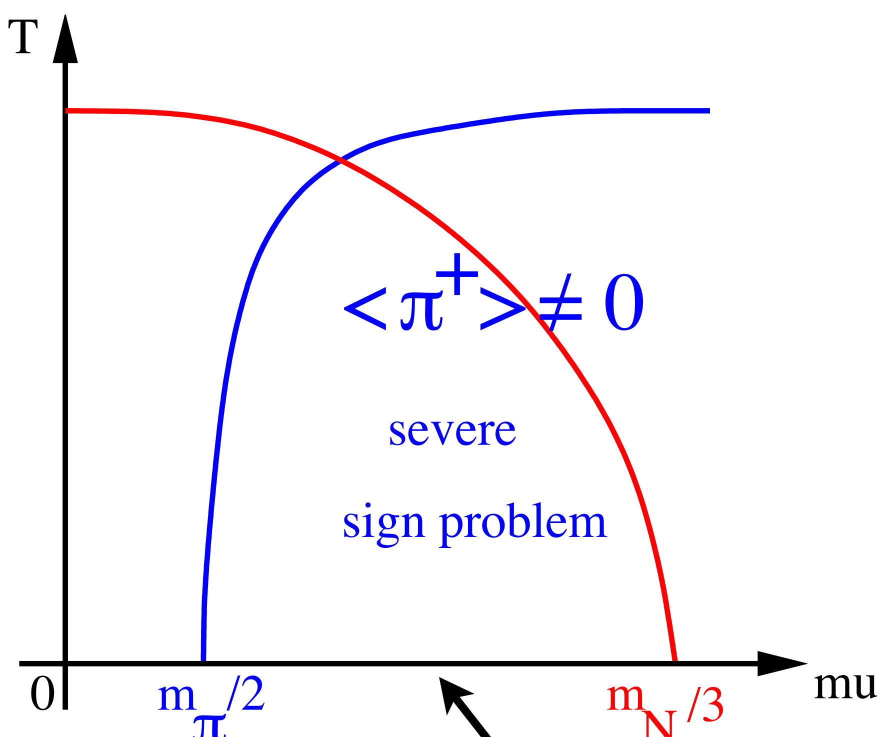
- av. sign $= \frac{Z_{\mathrm{QCD}}(\mu)}{Z_{|\mathrm{QCD}|}(\mu)} = e^{-\frac{V}{T}[f(\mu_u=+\mu,\mu_d=+\mu) - f(\mu_u=+\mu,\mu_d=-\mu)]}$ (for $N_f = 2$)



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

"Silverblaze pb": phase of det changes groundstate

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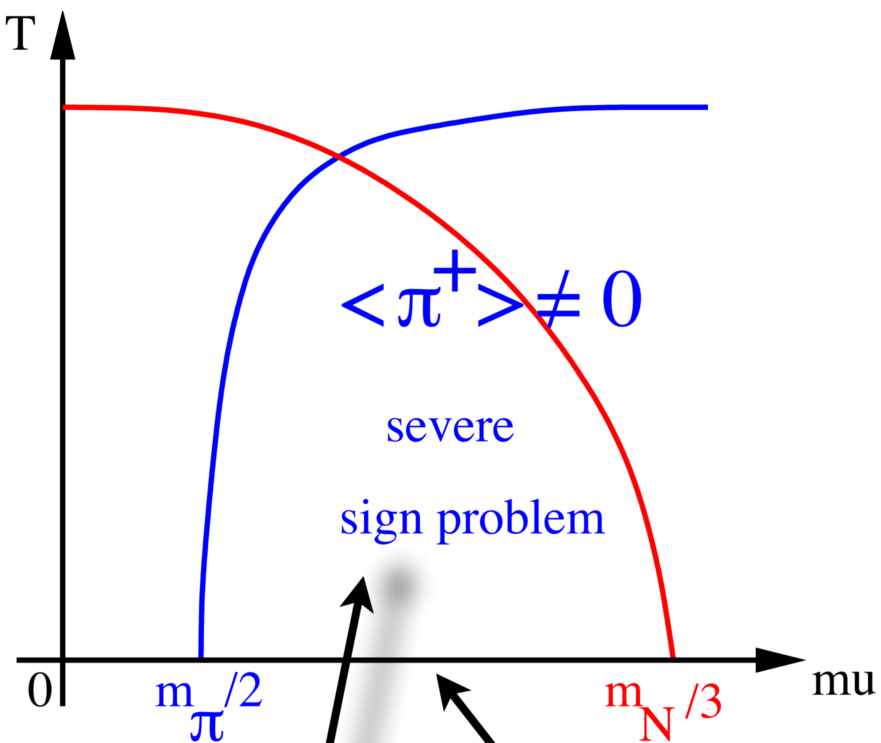

"Silverblaze pb": phase of det changes groundstate

Extremely hard

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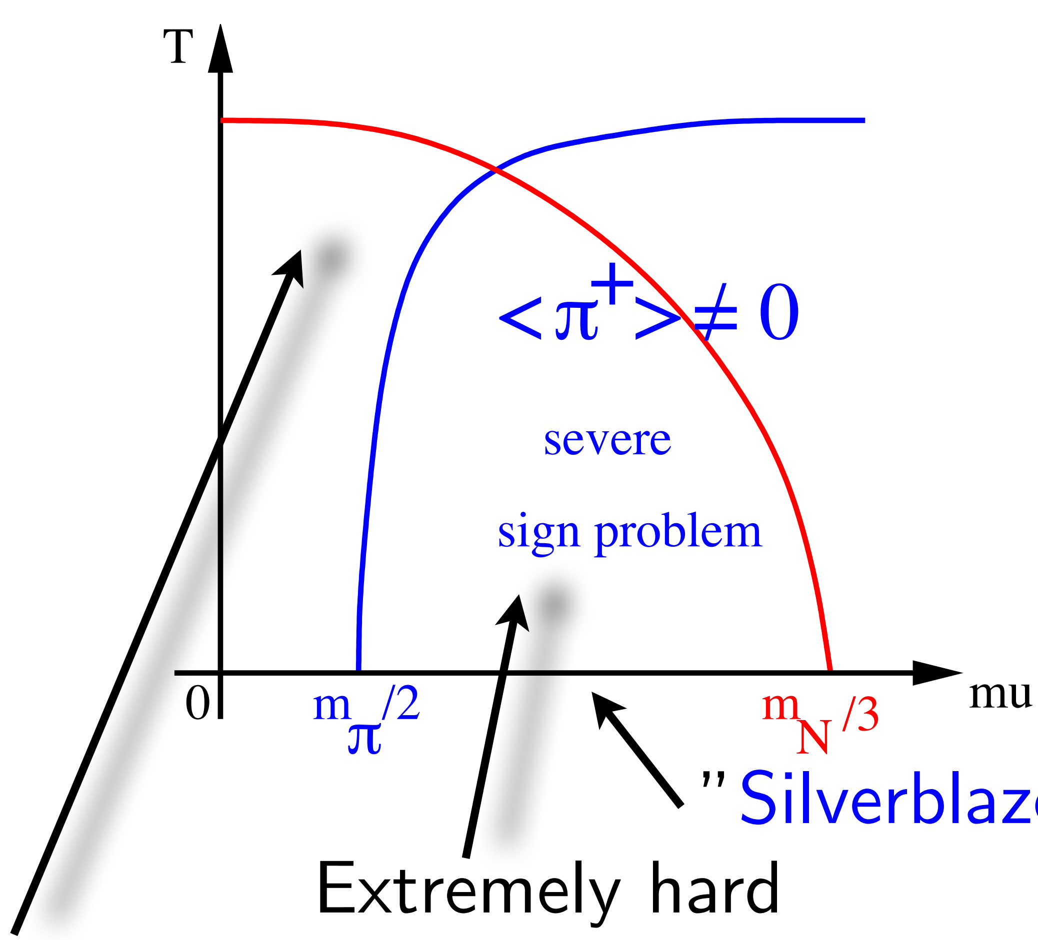


"Silverblaze pb": phase of det changes groundstate

Extremely hard

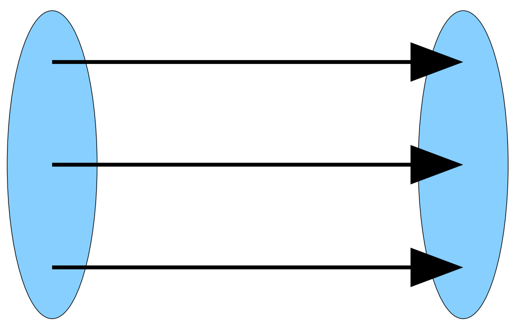
Not as hard
$\frac{\mu}{T} \lesssim 1$

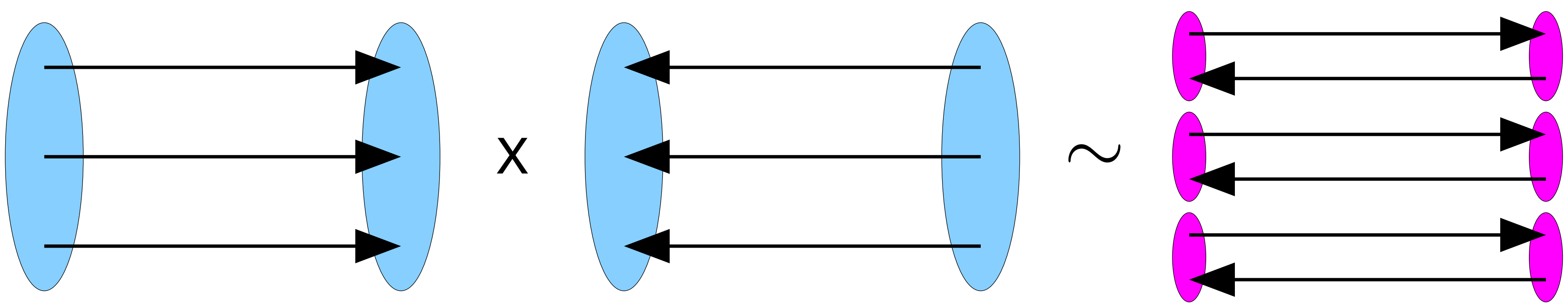
$\Delta f(\mu^2, T)$ large in the Bose phase
$\rightarrow$ "severe" sign pb.

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

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

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

- 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.)