The QCD phase diagram from the lattice

Philippe de Forcrand
ETH Zürich & CERN

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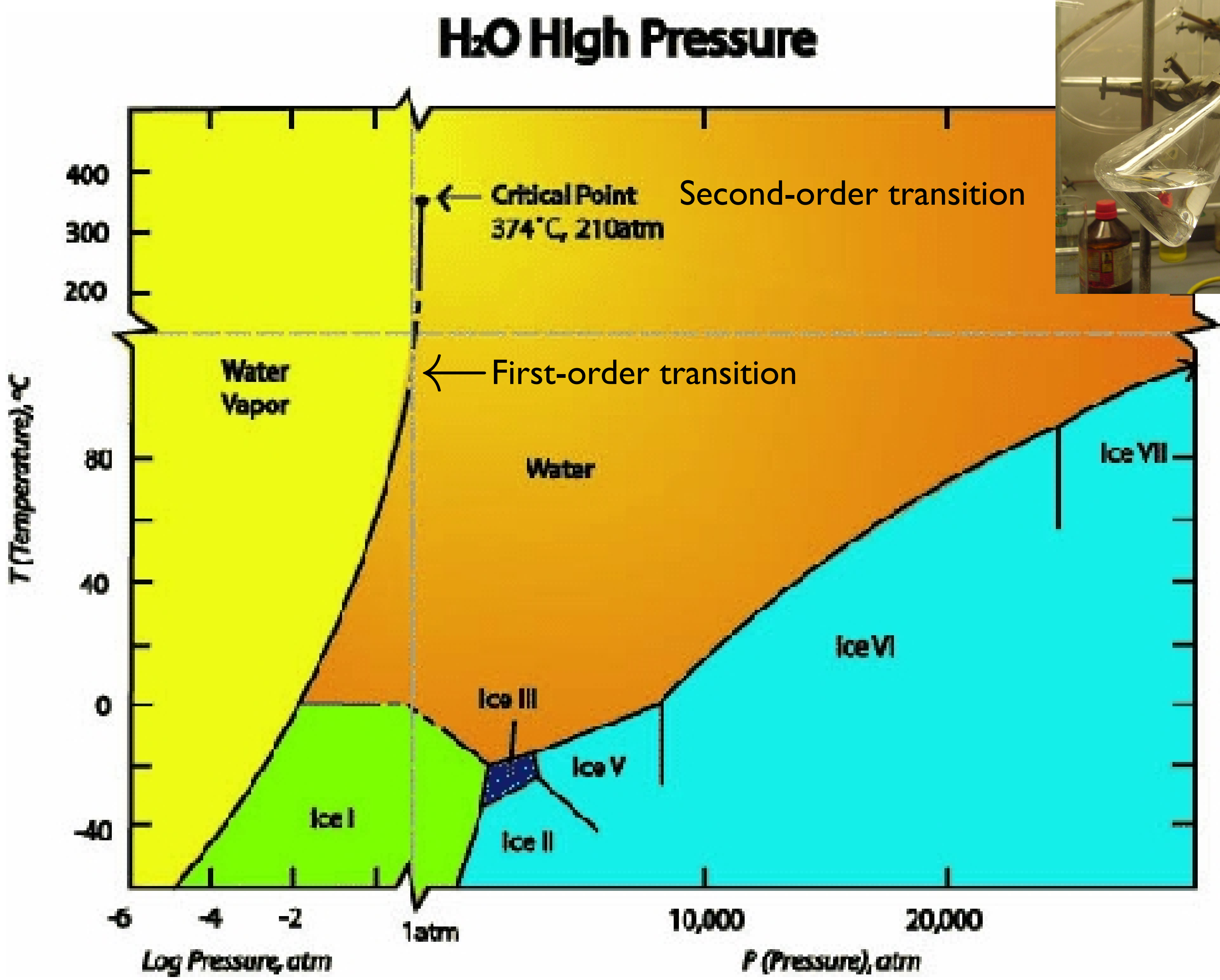
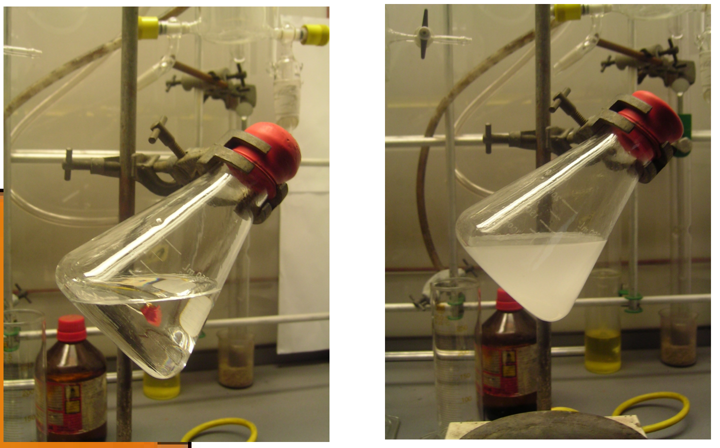
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Motivation

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

Water changes its state when heated or compressed



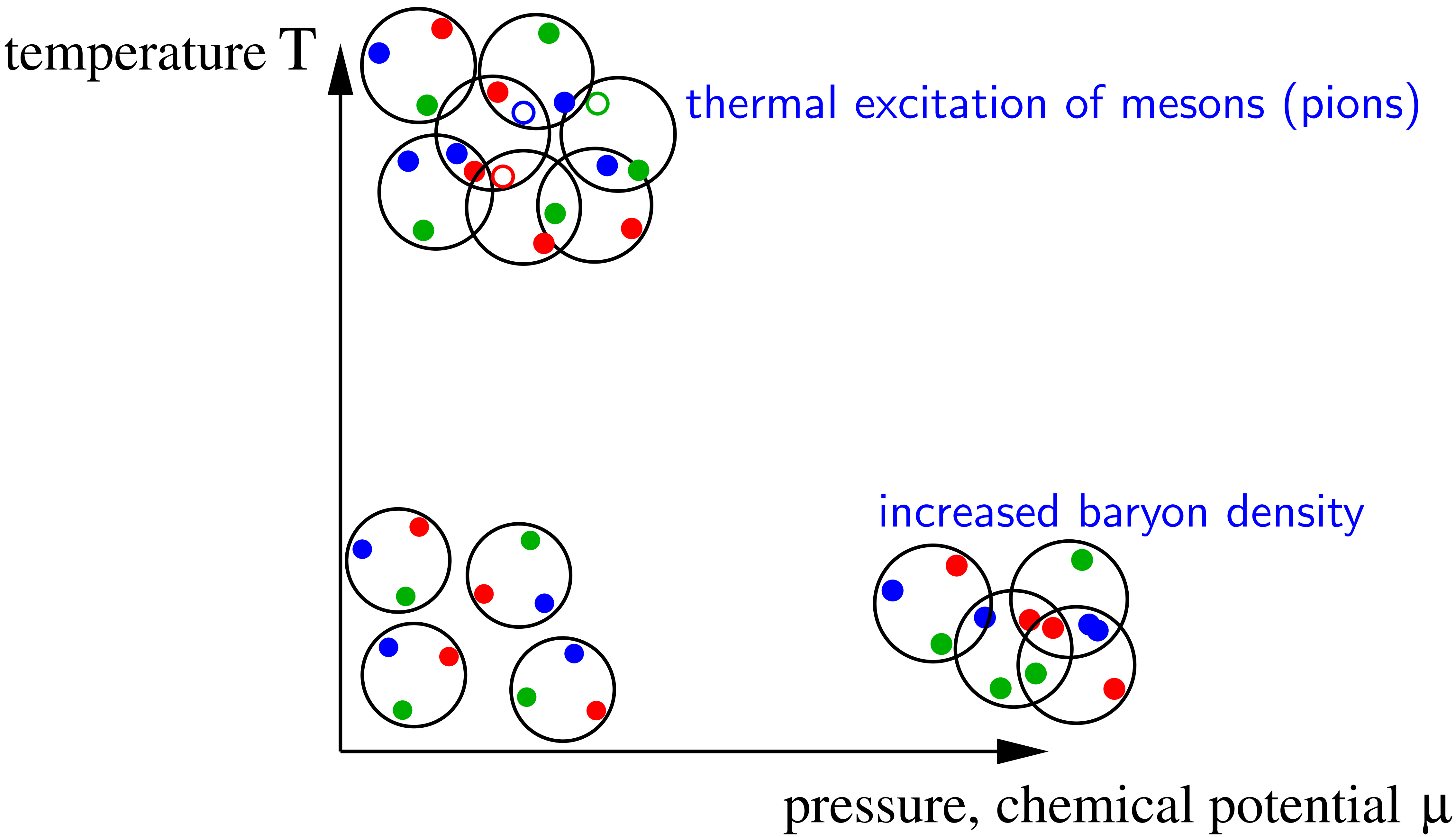


critical opalescence

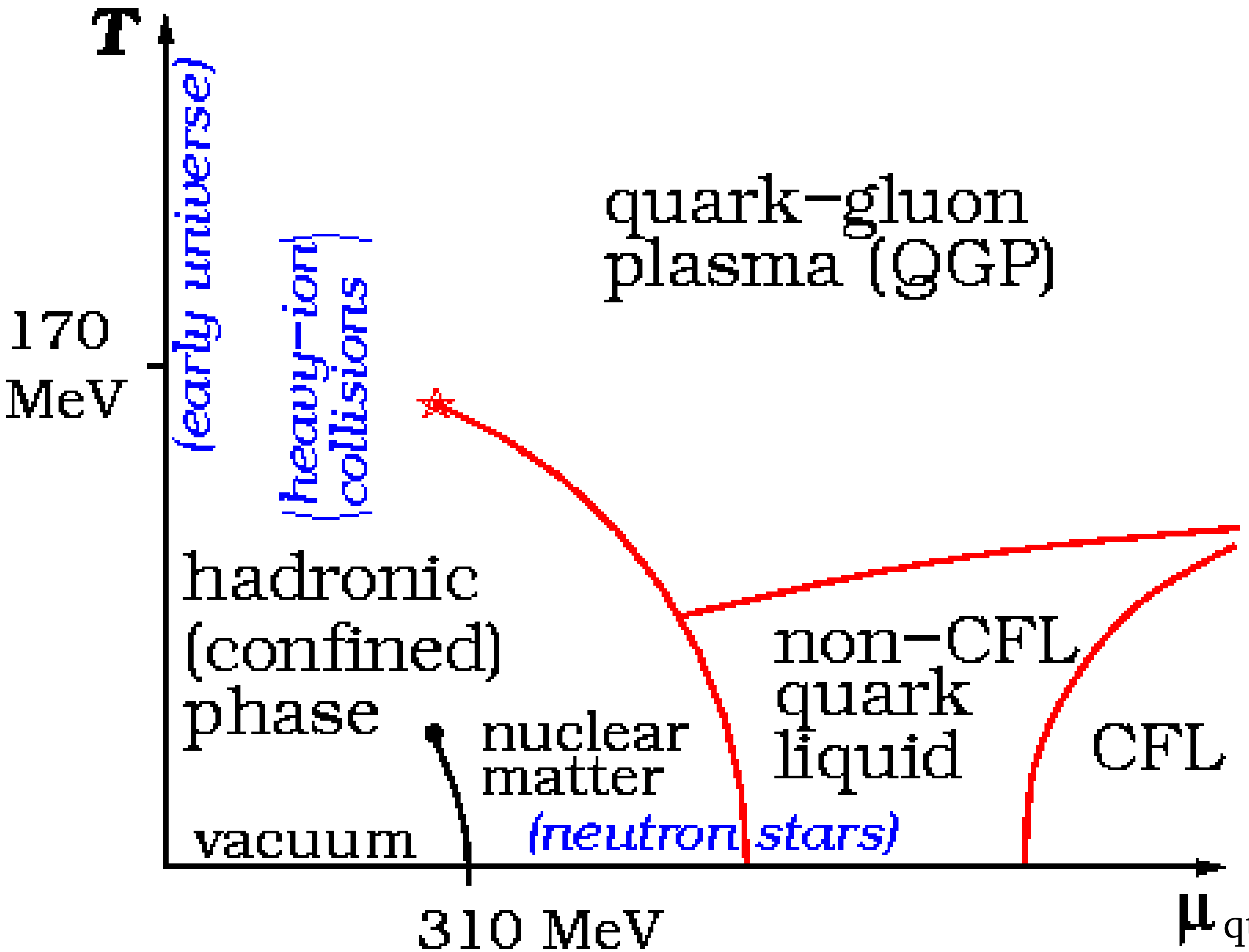
What happens to quarks and gluons when heated or compressed?

QCD under extreme conditions

Confinement: quarks are bound in color-neutral hadrons: qqq baryons & $q\bar{q}$ mesons
Compress or heat baryons: hadrons overlap → confinement "lost"
⇒ expect interesting/unusual behaviour



The wonderland phase diagram of QCD from Wikipedia



$\mu_{\text{quark}} = \frac{1}{3}\mu_{\text{Baryon}}$

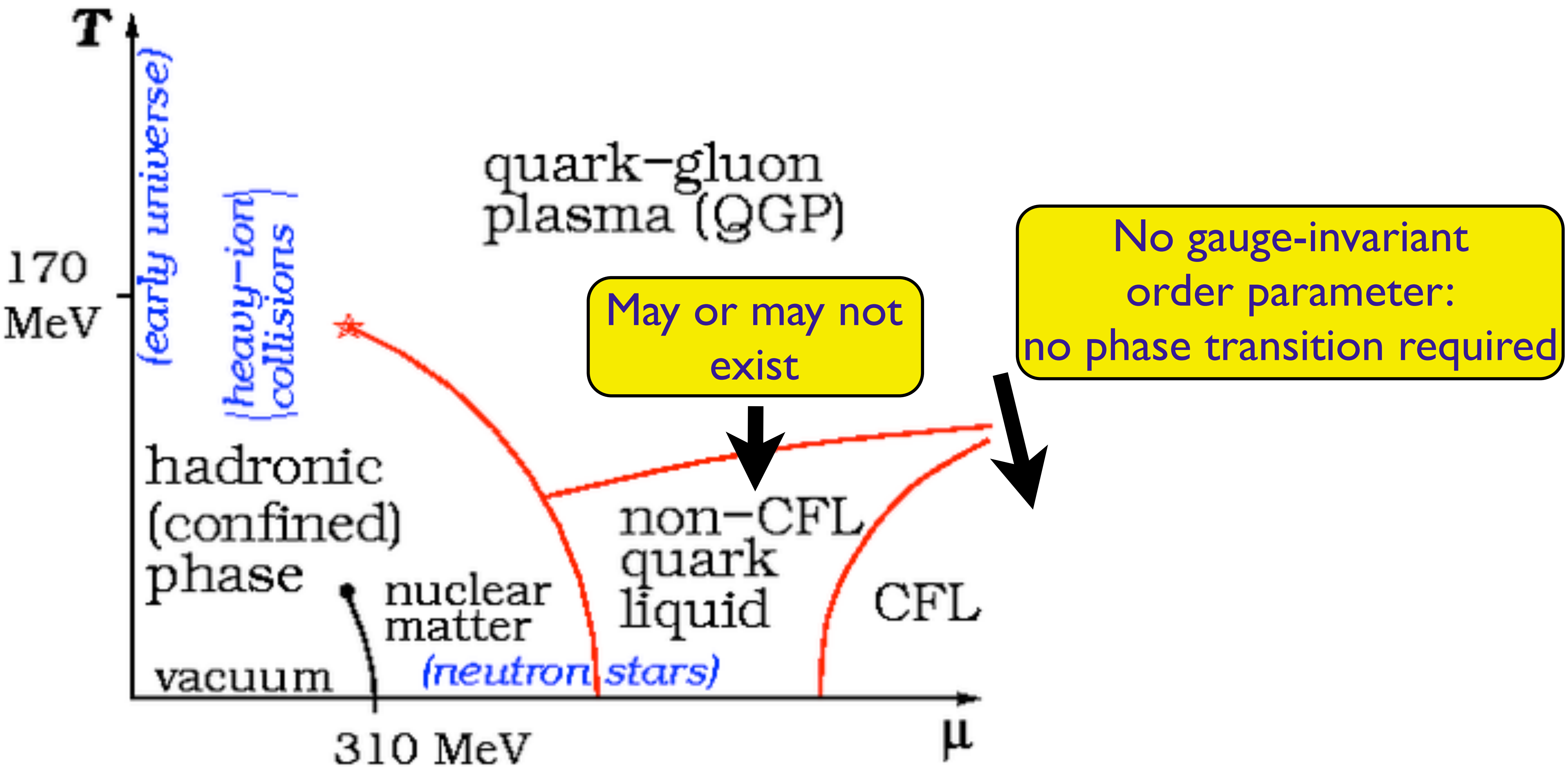
T or $\mu \to \infty$:
interaction weak
(asymptotic freedom)

Also:

- crystal phase(s)
- quarkyonic phase
- strangelets

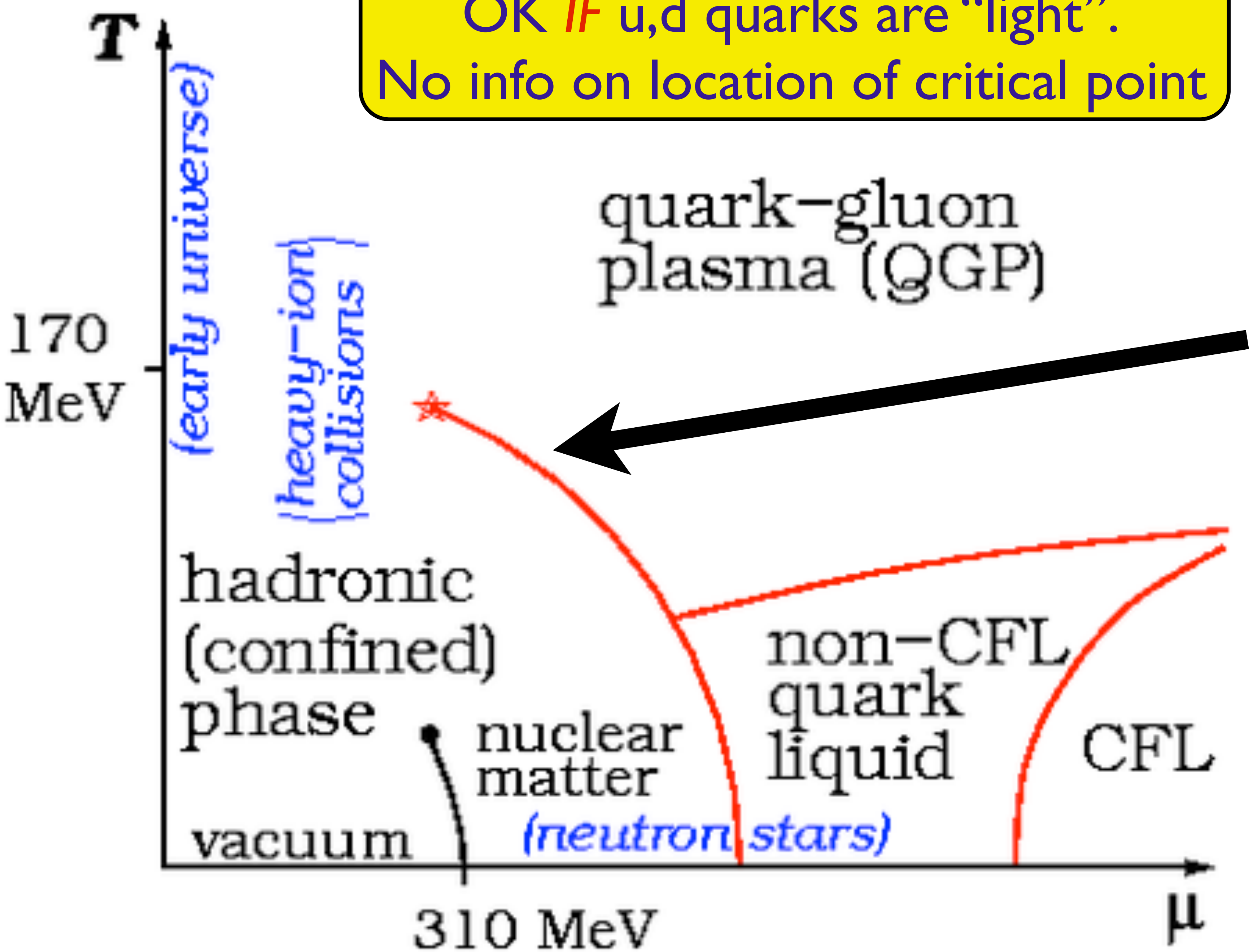
...

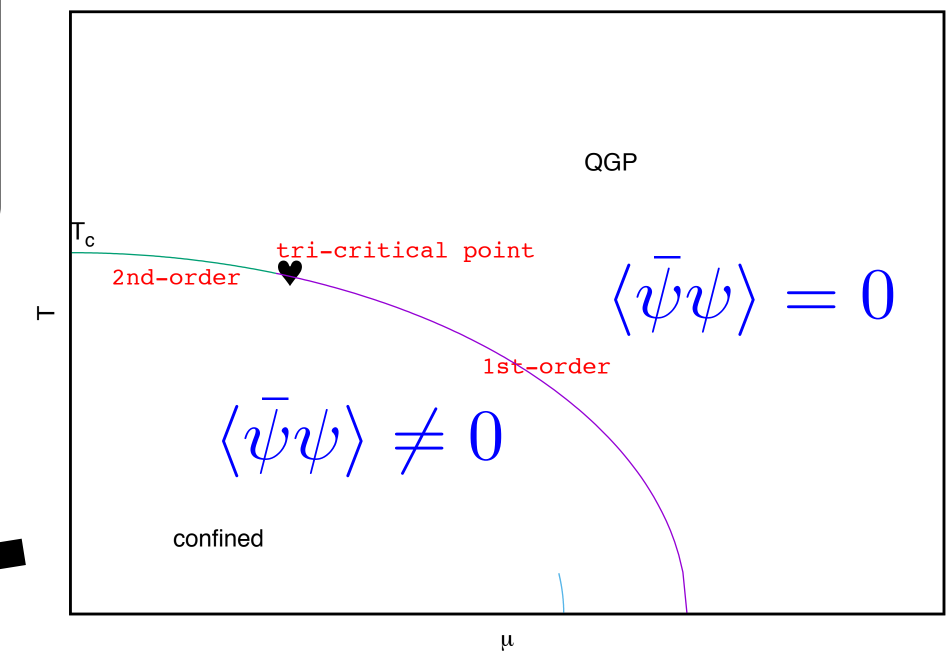
Caveat: everything in red is a conjecture


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

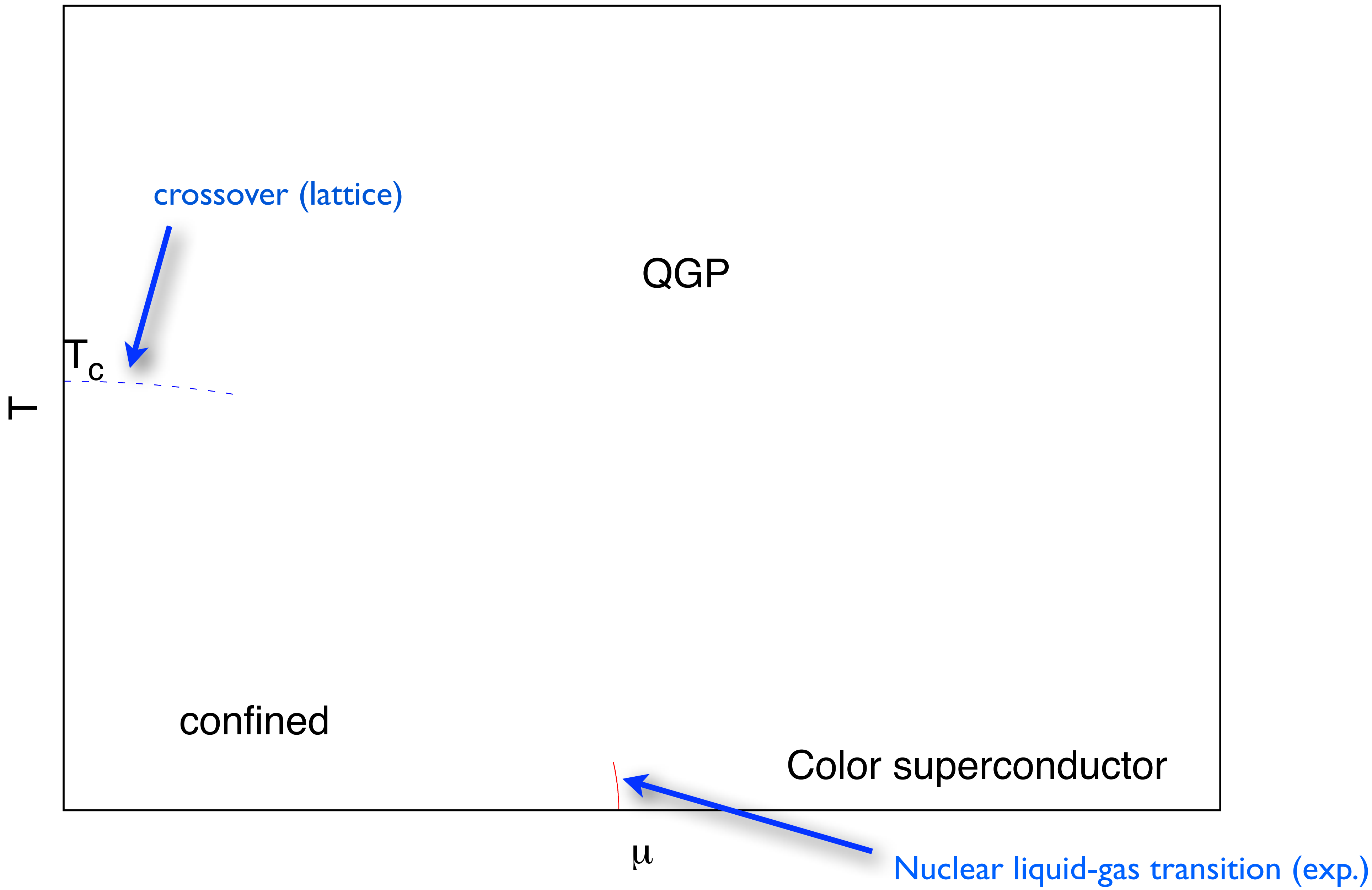
$N_f = 2, m_u = m_d = 0$





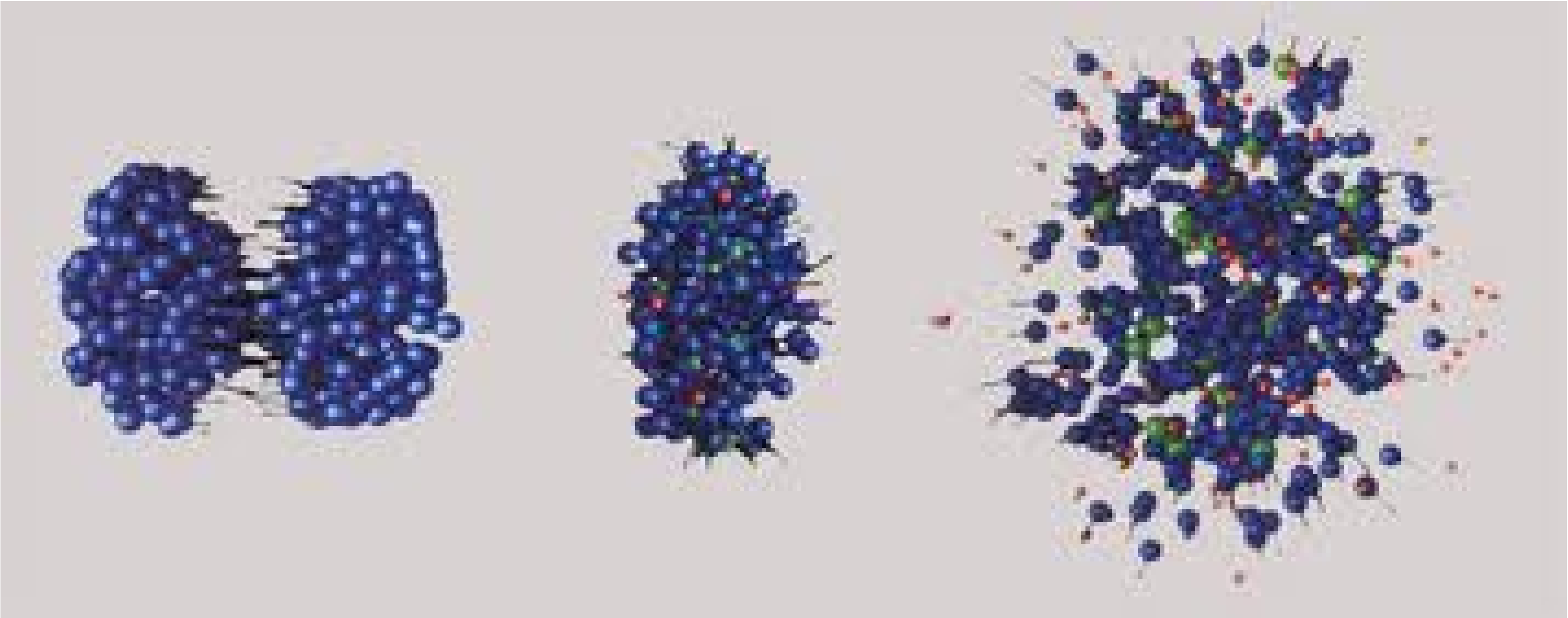
Finite μ: what is known?

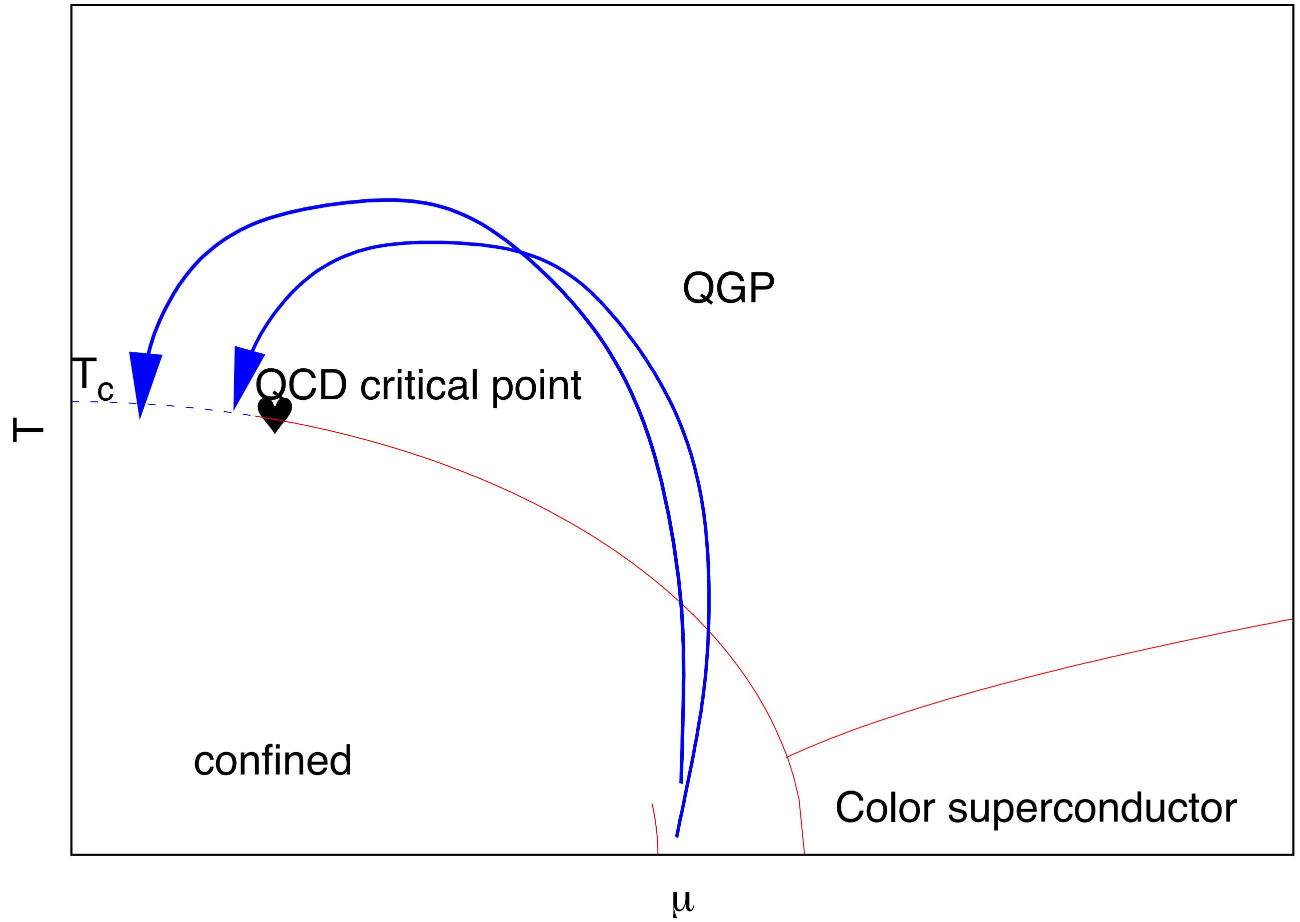
really



Minimal, possible phase diagram

Heavy-ion collisions





Knobs to turn:

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

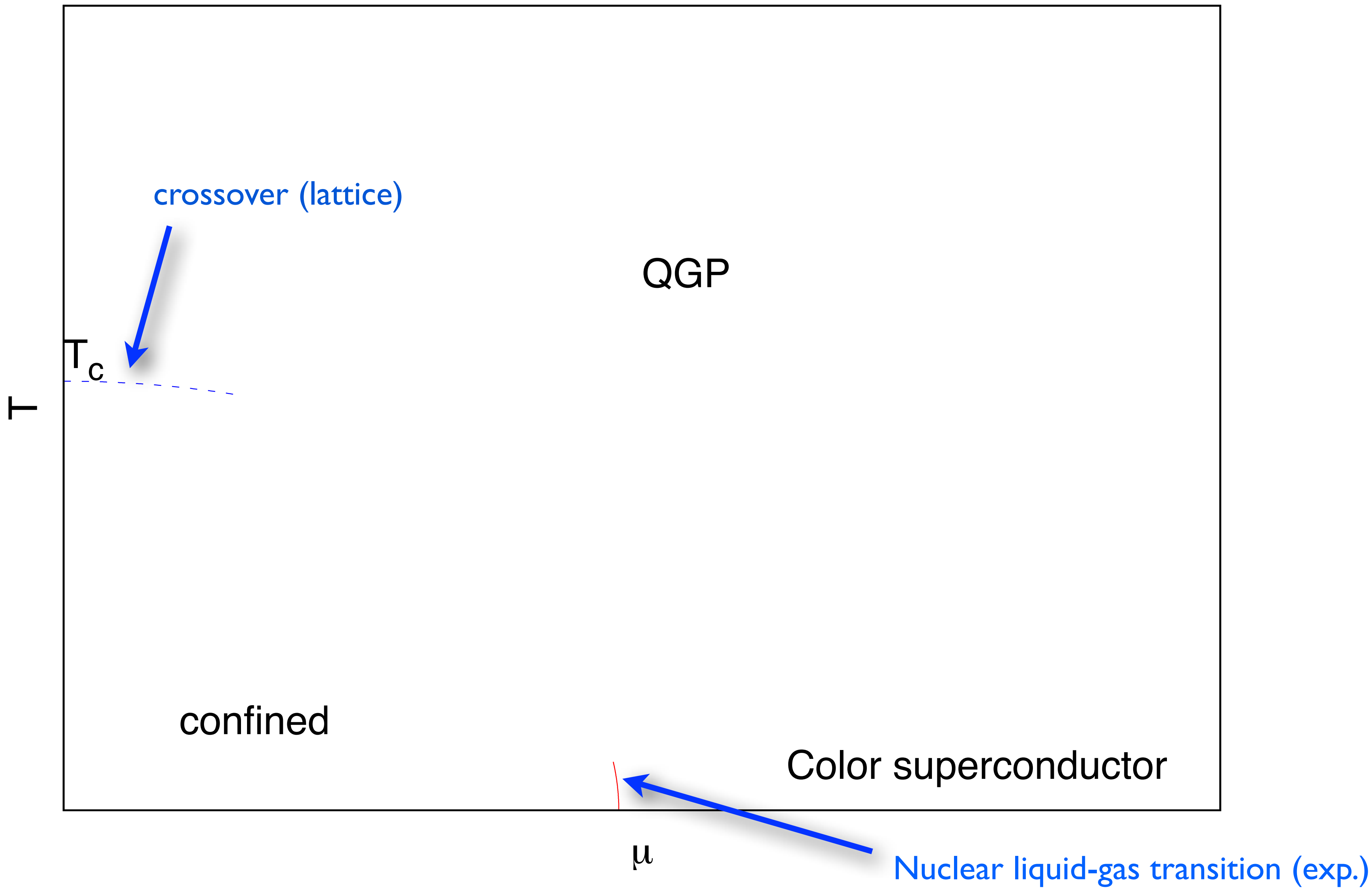
So far, no sign of QCD critical point
(esp. RHIC beam energy scan)

"critical opalescence" ?

non-Gaussian fluctuations (Stephanov)

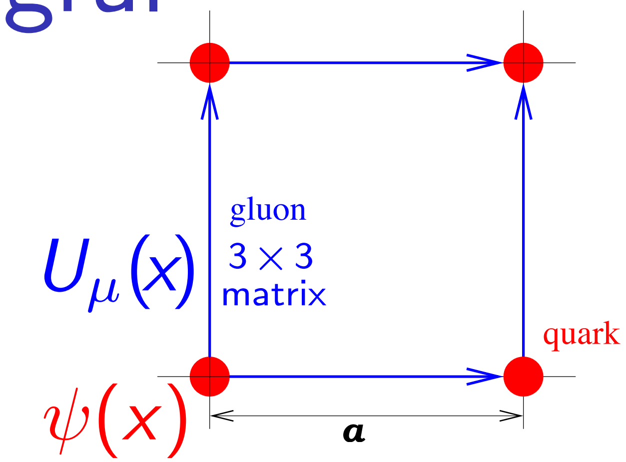
Finite μ: what is known?

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



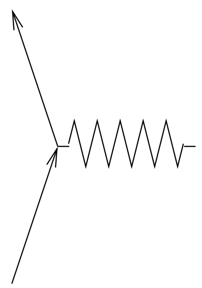
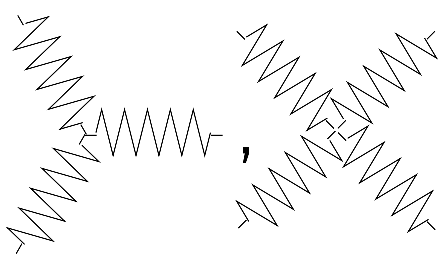
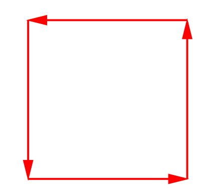
Minimal, possible phase diagram

Lattice QCD: Euclidean path integral



space + imag. time → $4d$ 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 $\bar{\psi}\not{D}\,\psi$
  -  $\longrightarrow$ β ReTrU_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) → determinant *non-local*

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

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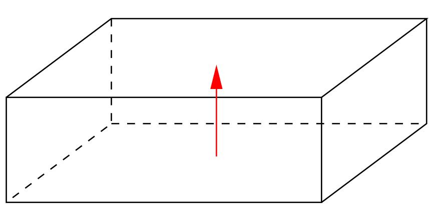
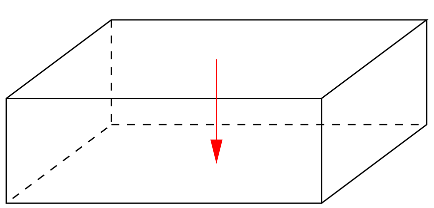
- Measure $d\varpi \sim \det \not{D}$ *must be complex* to get correct physics:



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



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$$\mu \neq 0 \Rightarrow F_q \neq F_{\bar{q}} \Rightarrow \mathrm{Im} d\varpi \neq 0$$

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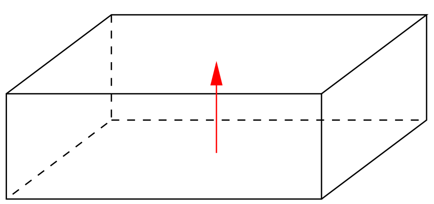

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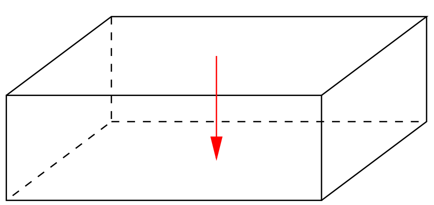

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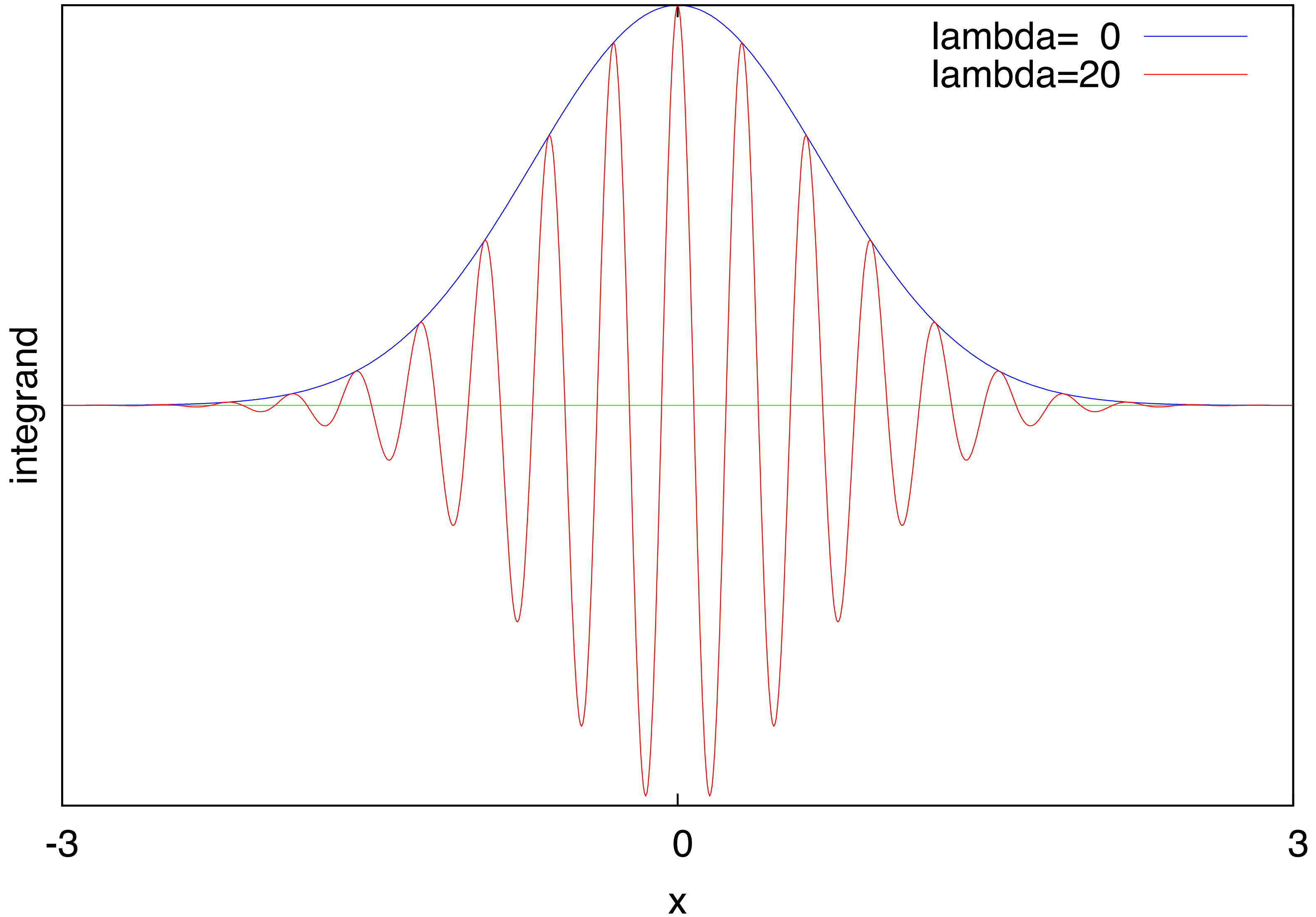
- Origin: $\mu \neq 0$ breaks charge conj. symm., ie. usually complex conj.

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

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

  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.

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

$\longrightarrow$ "Sign problem" conferences...

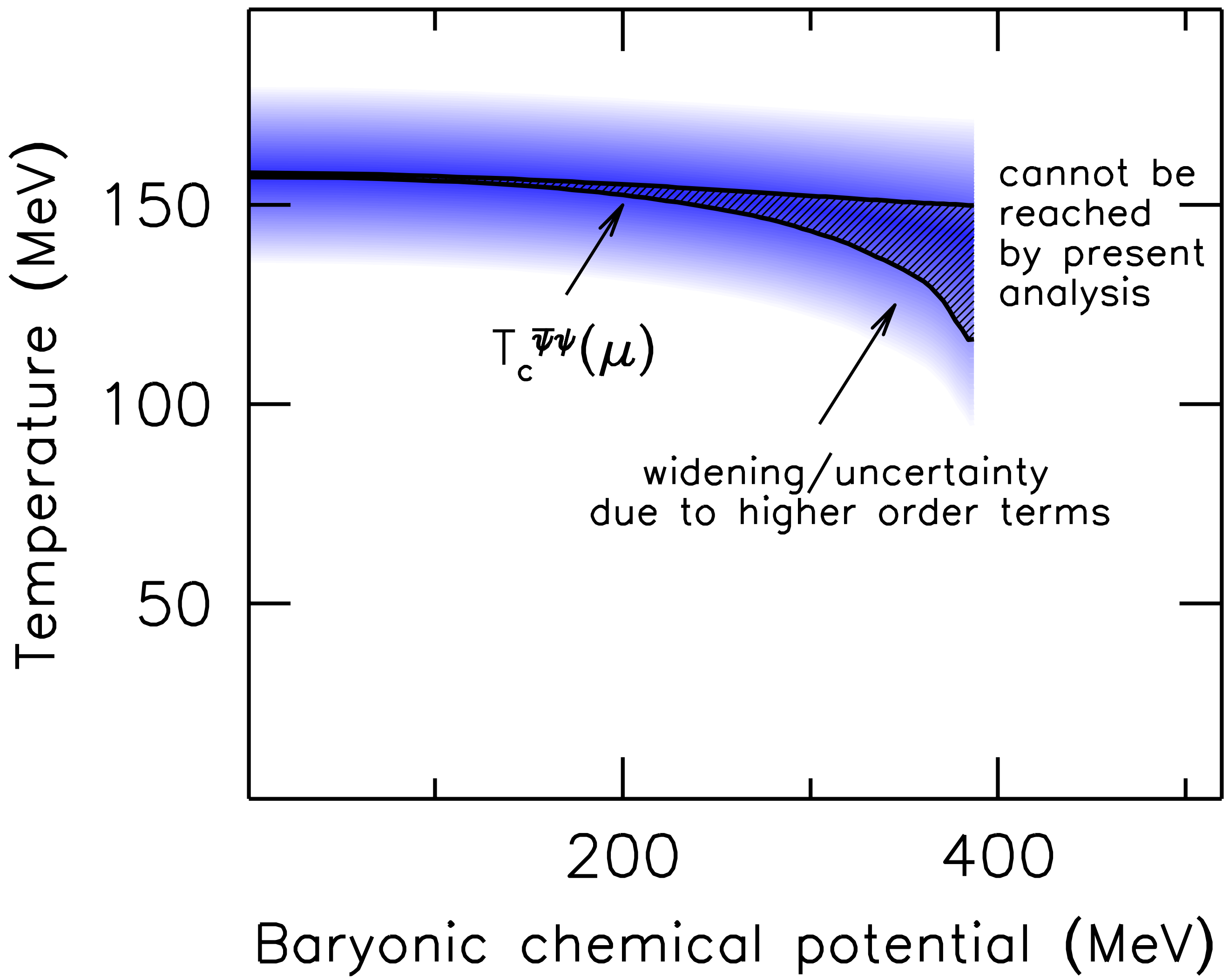
First frog steps: $\frac{\mu}{T} \lesssim 1$

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

- 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.



Steve Weinberg's
Third Law of Progress in Theoretical Physics

You may use any degrees of freedom you like to describe a physical system,
but if you use the wrong ones, you'll be sorry

in "Asymptotic realms of physics", 1983

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Optimal choice: Monte Carlo on physical states *(no sign pb)*

- ★ Integrate out quarks, then Monte Carlo on gluons: *Not good (sign pb)*
- ★ Integrate out gluons, then Monte Carlo on color singlets: *Much better*

like physical states

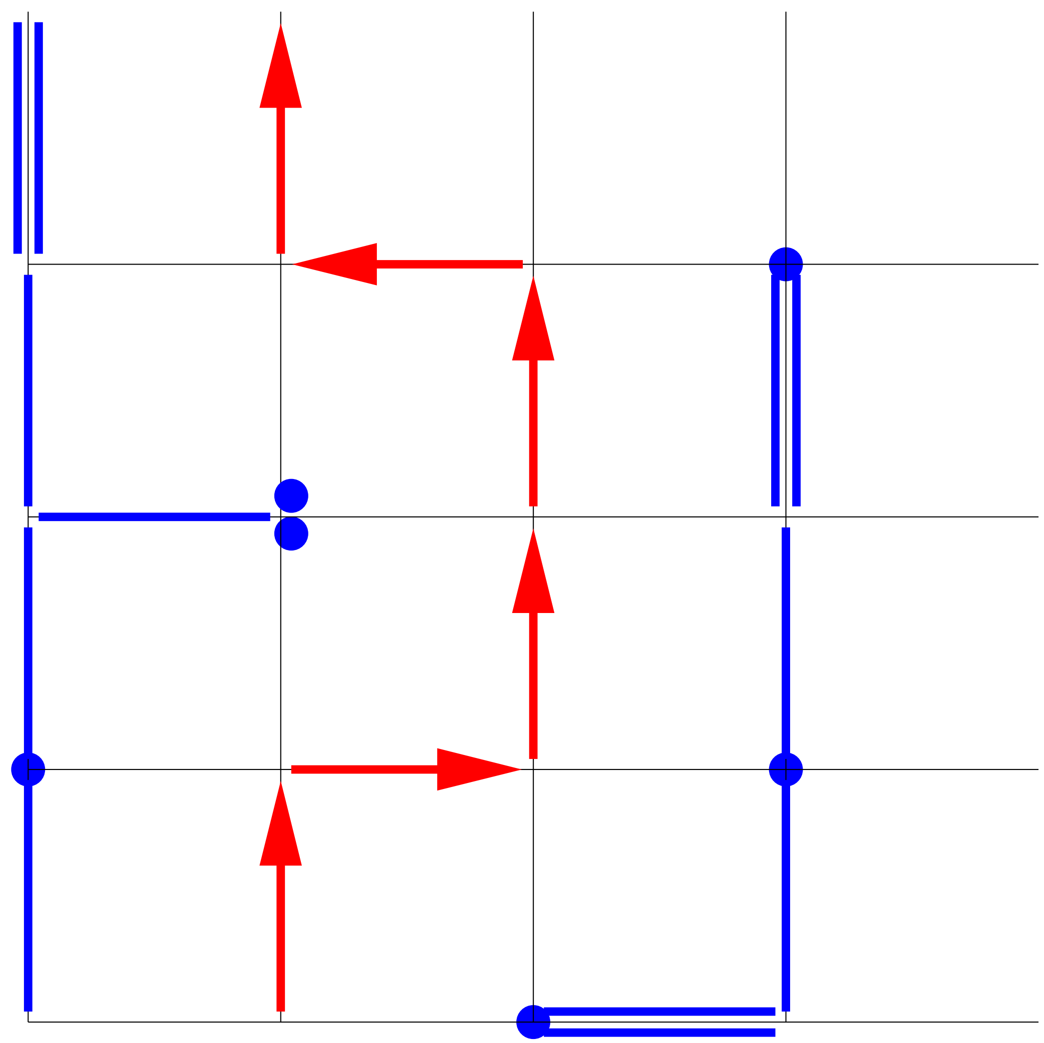
Easy at strong coupling $\beta = \frac{6}{g_0^2} = 0$: 4-link interaction $\beta \, \mathrm{ReTr} U_P$ drops out

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 ($\bullet$ $\bar{\psi}\psi$, meson hop)
or a baryon loop

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

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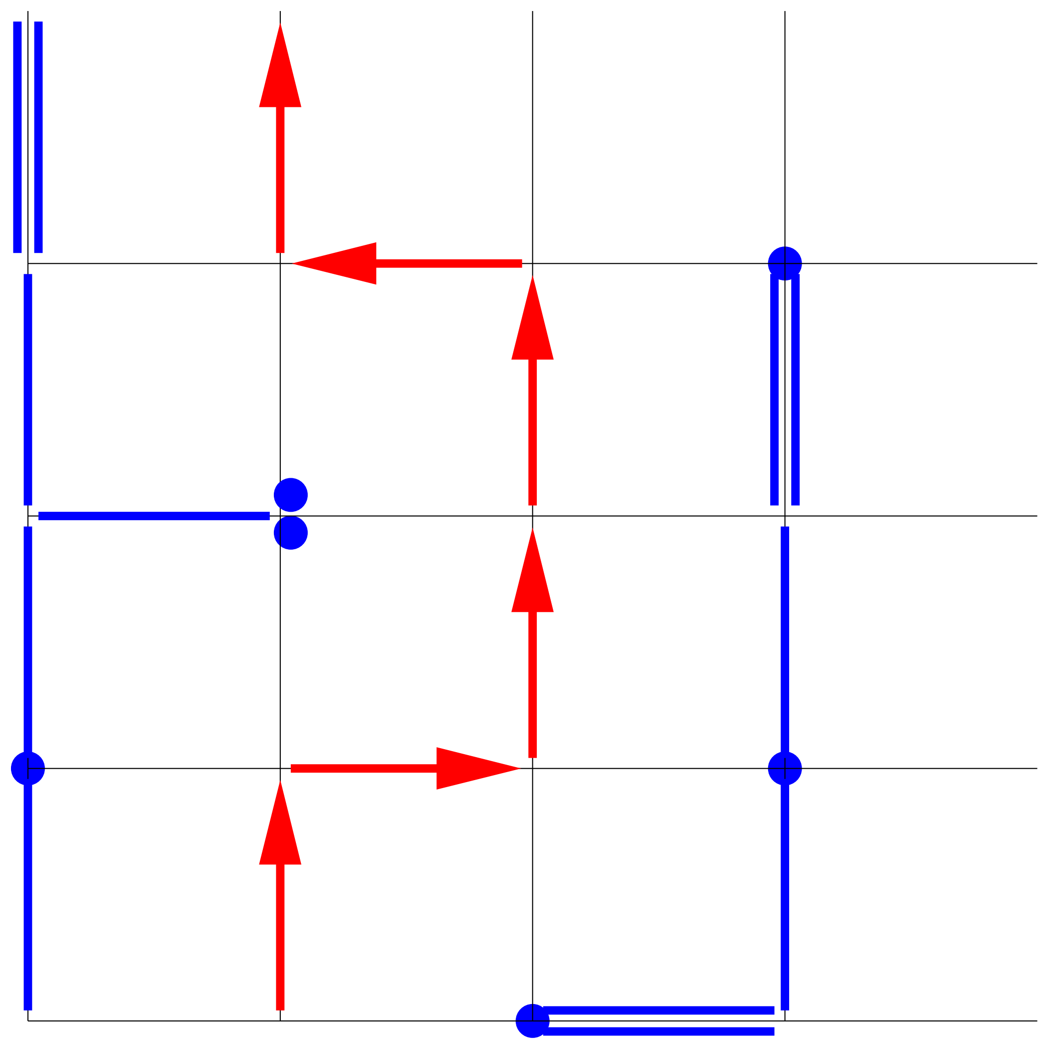

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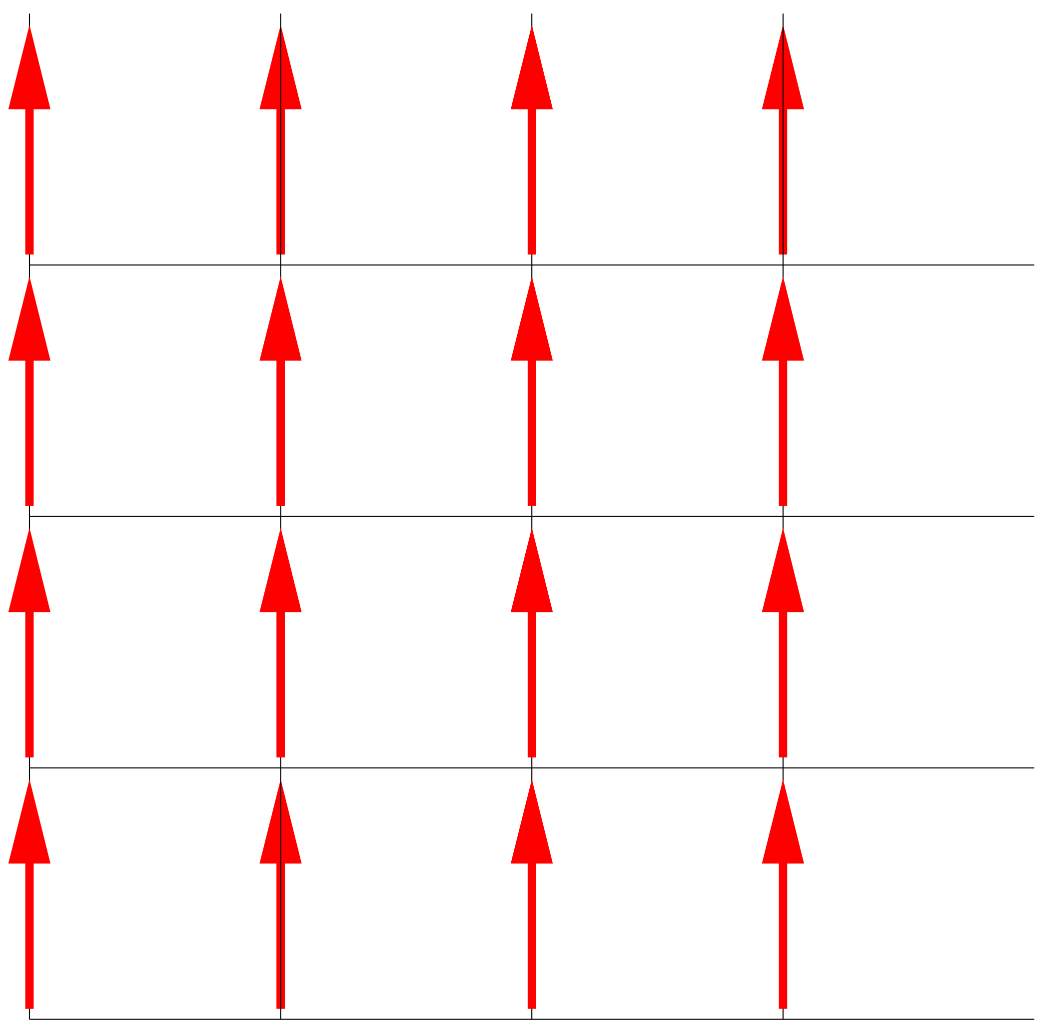


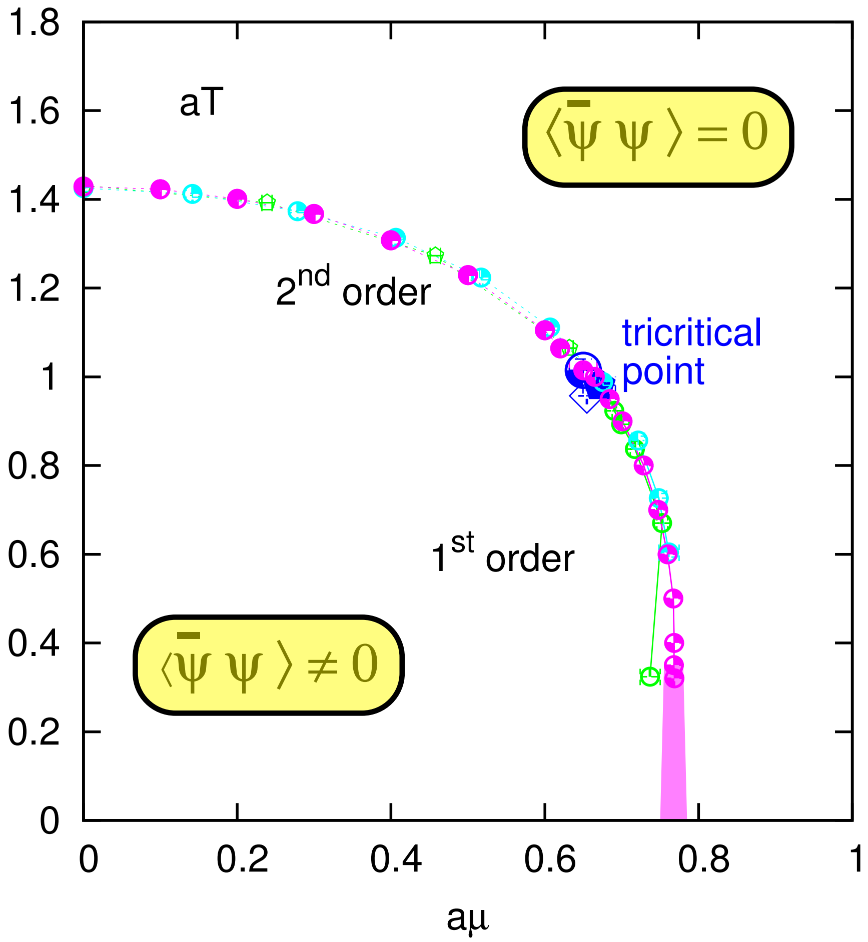
The dense (crystalline) phase:
1 baryon per site; no space left
$\rightarrow \quad \langle\bar{\psi}\psi\rangle = 0$

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

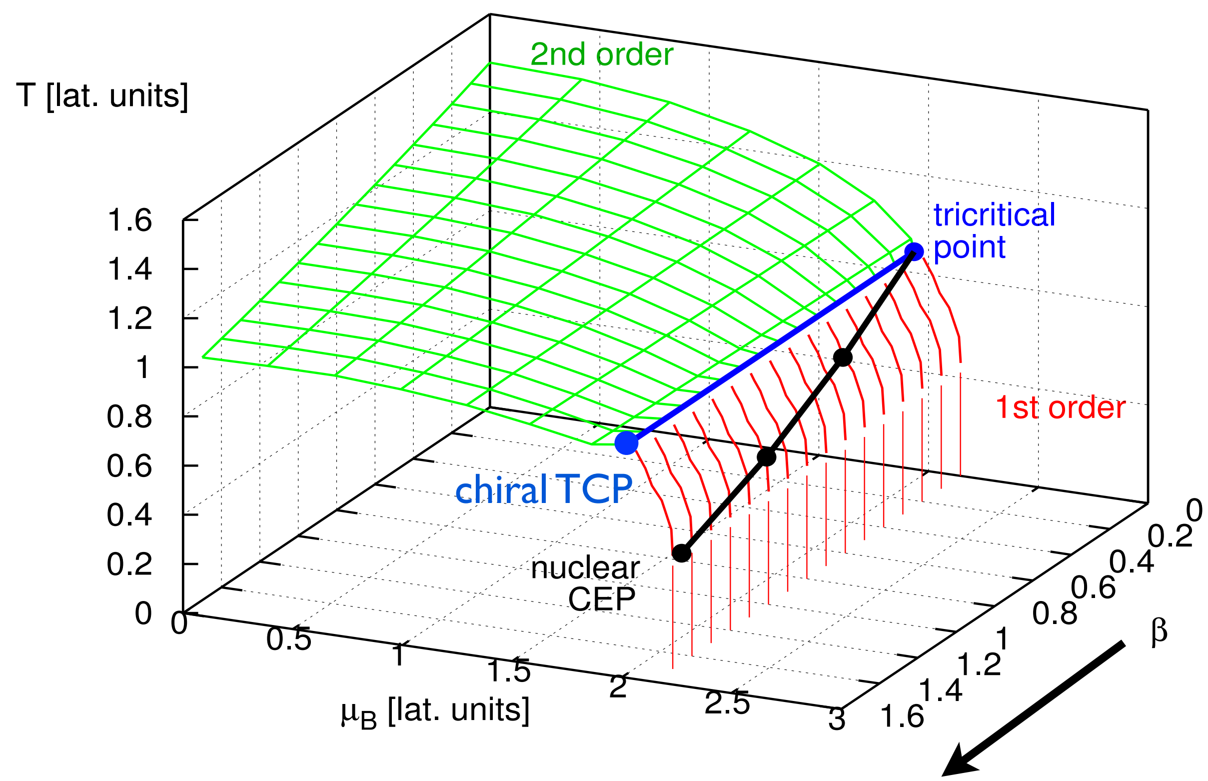
Results $\beta \approx 0$ w/Unger, Langelage, Philipsen

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

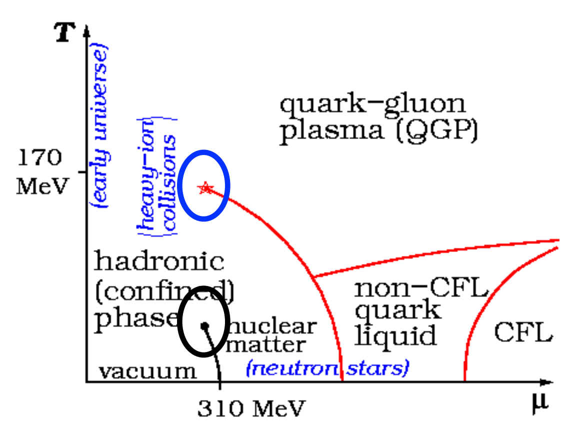
$\beta = 0$



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



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



Conclusions

- QCD phase diagram: possibly rich -- or not

- QCD critical point: *not at small chem. pot.*

- Sign problem: hot, interdisciplinary topic

Remember: Corfu is home of Princess Nausicaa, one of the few women with whom Odysseus did ***not*** reach a critical point...

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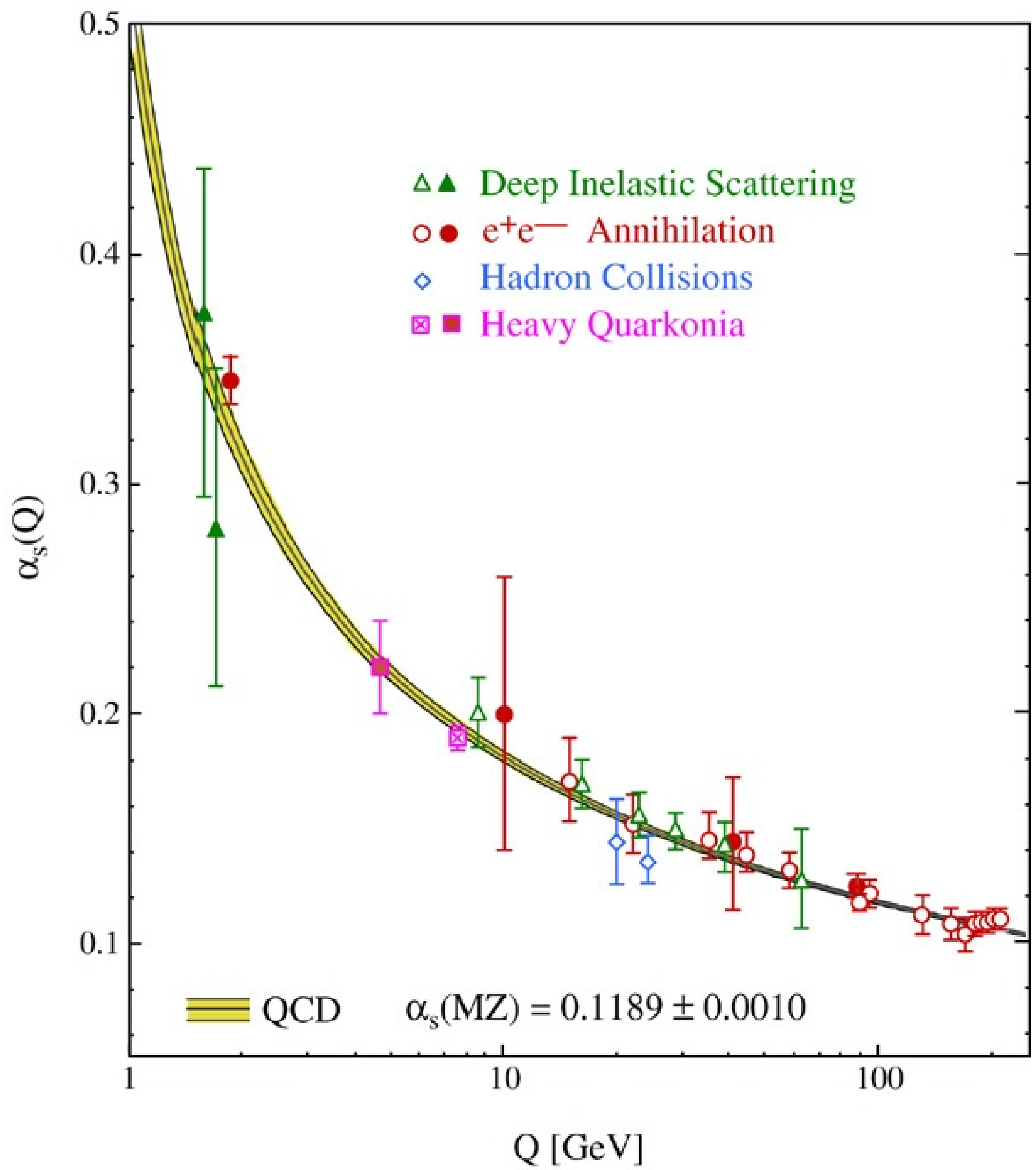
- Second Law: do not trust arguments based on lowest-order perturbation theory

- First Law: you will get nowhere by just churning equations

Basic properties of QCD

- QCD describes properties of *quarks* (cf. electrons – fermions)
  interacting by exchanging *gluons* (cf. photons – bosons)

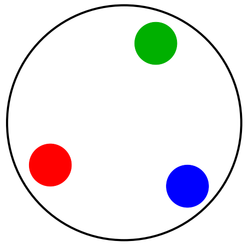
- QCD is *asymptotically free*: weaker interaction at higher energy



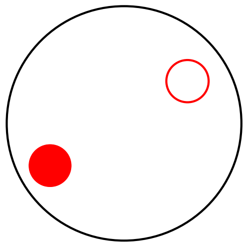
The flip side of asymptotic freedom: "infrared slavery"

- 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, ...

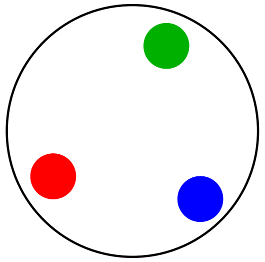


Exotics: glueballs, tetraquarks $qq\bar{q}\bar{q}$, pentaquarks $qqqq\bar{q}$, etc...

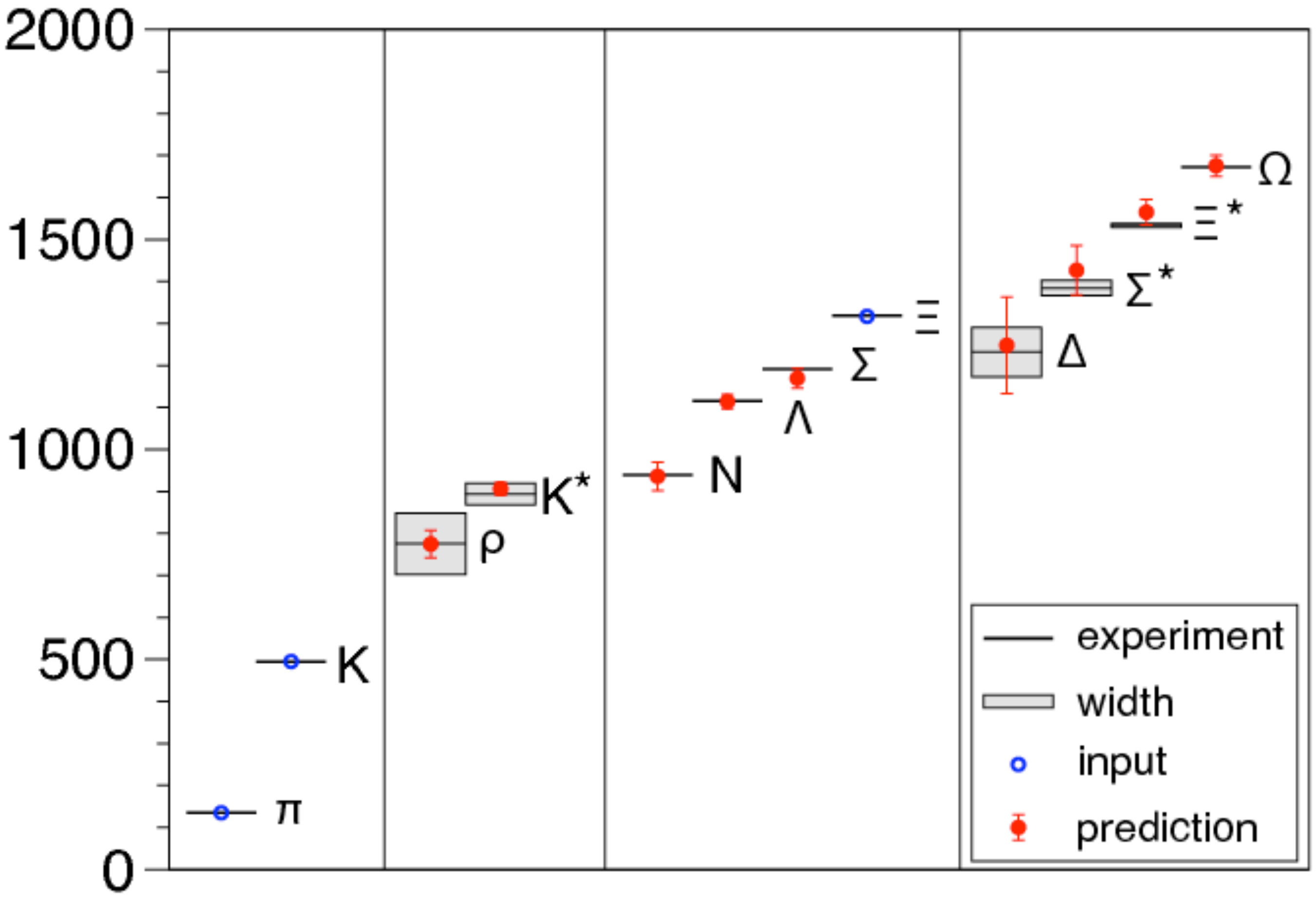
In principle, all calculable by Lattice QCD simulations

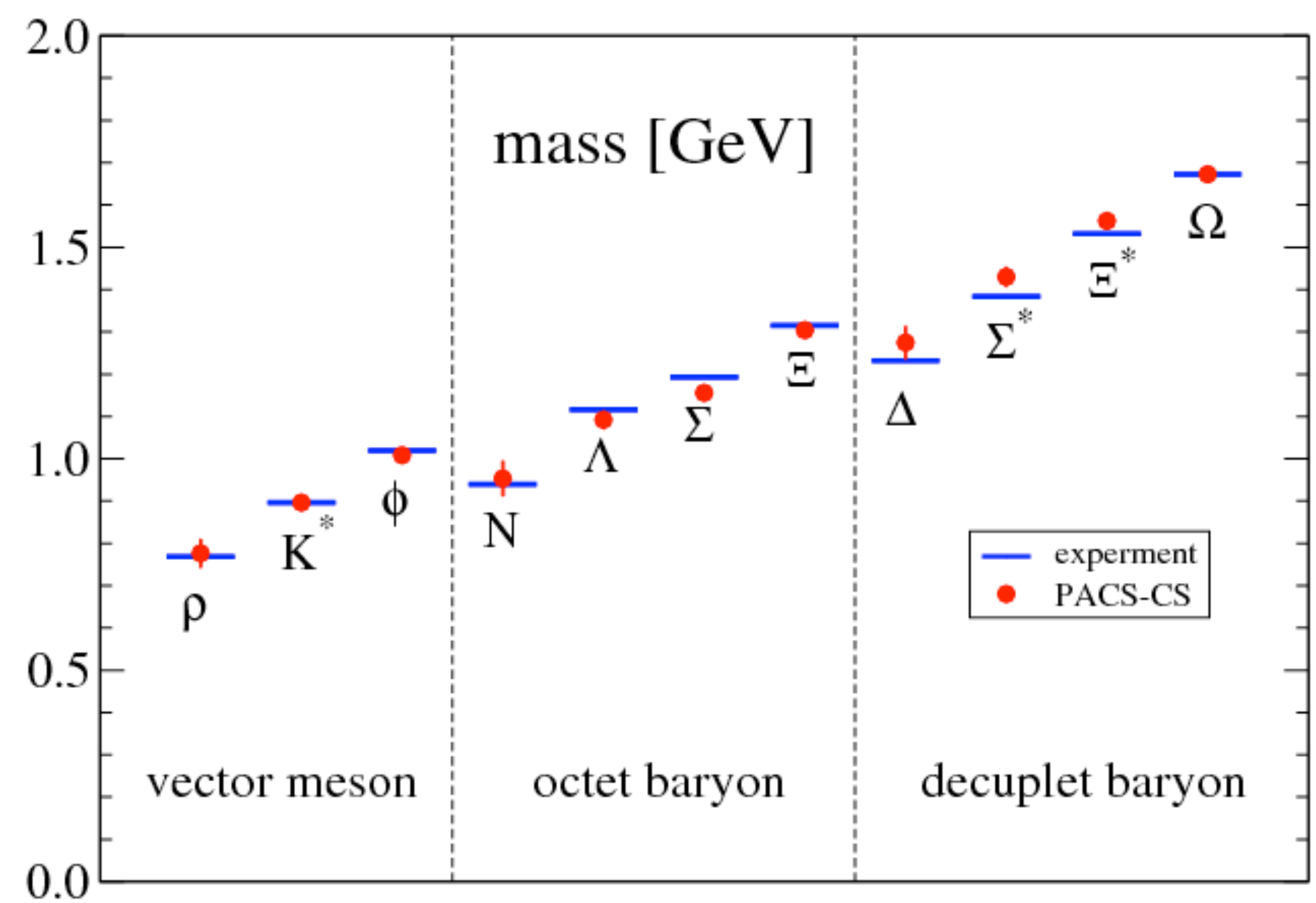
Scope of lattice QCD simulations: Physics of color singlets

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



Example: hadron masses





BMW collaboration

arXiv:0906.3599 ⟶ Science

PACS-CS collaboration

arXiv:0807.1661

Follow-up: neutron-proton mass diff.

arXiv:1406.4088 ⟶ Science

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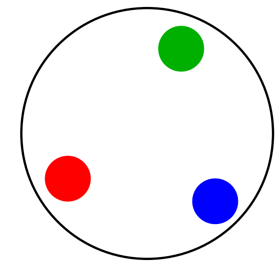
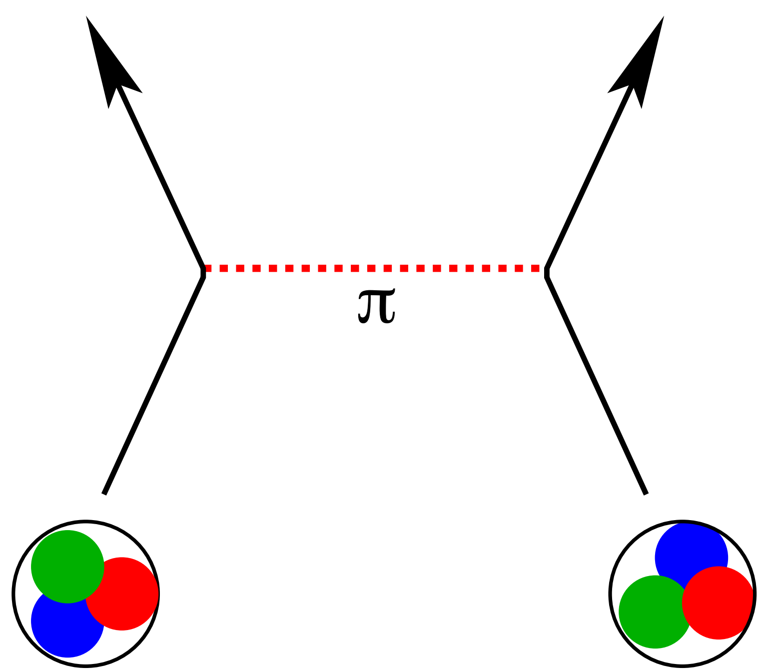


** "Two-body" physics: nuclear interactions
pioneers Hatsuda et al, Savage et al



hard-core
+
pion exchange?

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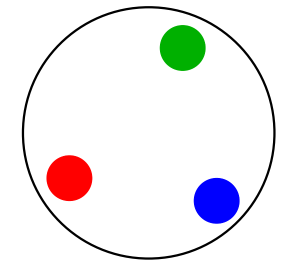

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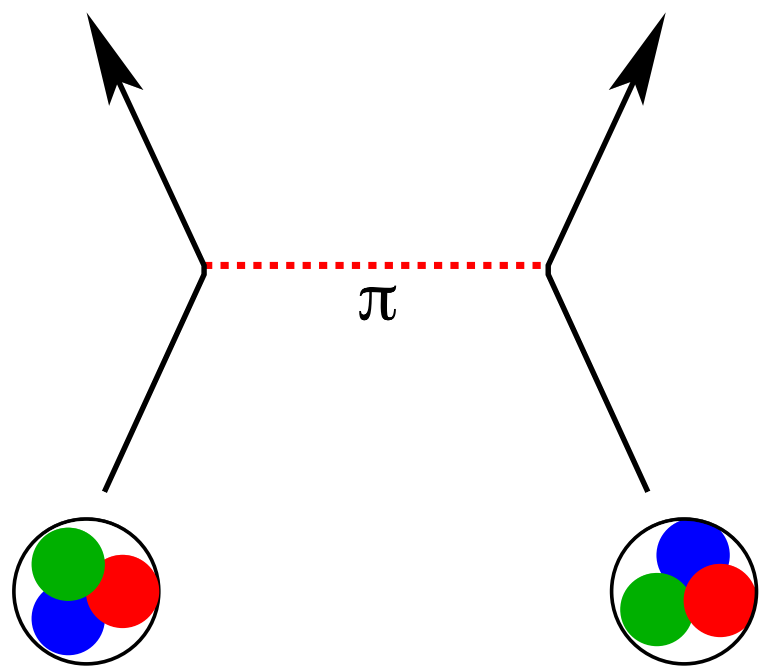

hard-core
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*** Many-[composite]-body physics: nuclear matter
phase diagram vs (temperature T, density $\leftrightarrow \mu_B$)

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 $\langle\psi_k|e^{-\frac{\beta}{N}H}|\psi_l\rangle = e^{-\frac{\beta}{N}E_k}\delta_{kl} \geq 0 \rightarrow$ no sign pb

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  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 $\langle\psi_k|e^{-\frac{\beta}{N}H}|\psi_l\rangle = e^{-\frac{\beta}{N}E_k}\delta_{kl} \geq 0 \rightarrow$ no sign pb

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

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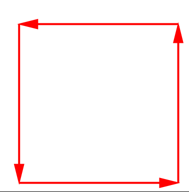
Usual:
- integrate over quarks analytically $\rightarrow \det(\{U\})$
- Monte Carlo over gluon fields $\{U\}$

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

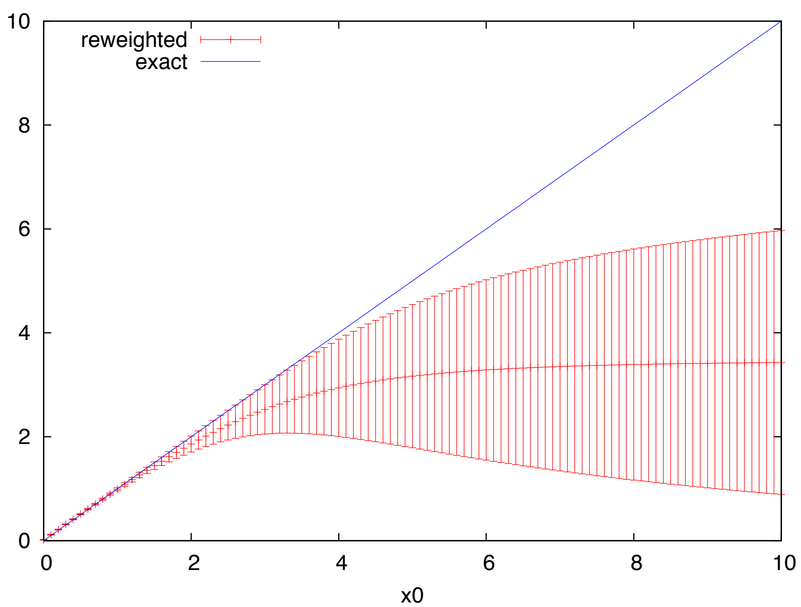
More difficulties: the overlap problem

- Further danger: insufficient overlap between sampled and reweighted ensembles

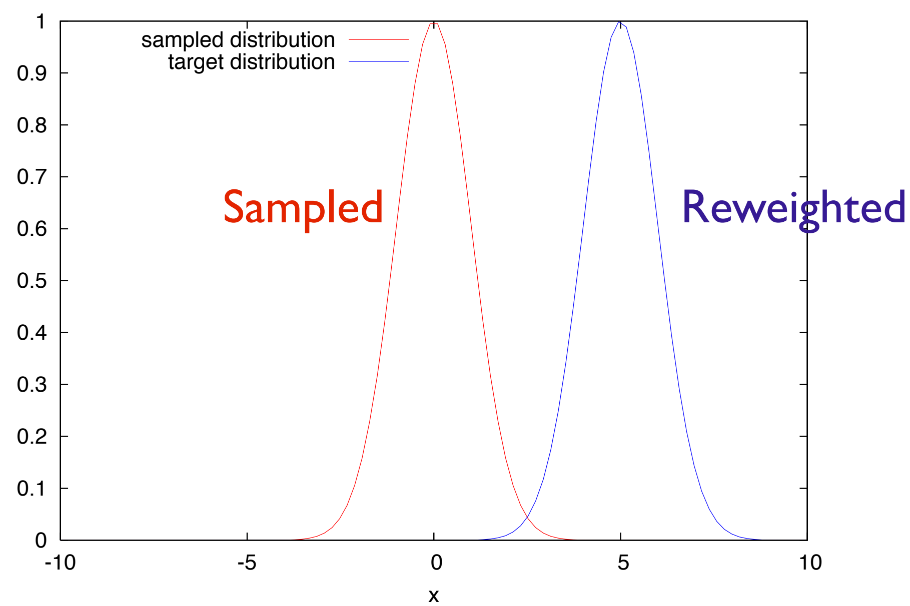
Very large weight carried by very rarely sampled states

$\rightarrow$ WRONG estimates in reweighted ensemble for finite statistics

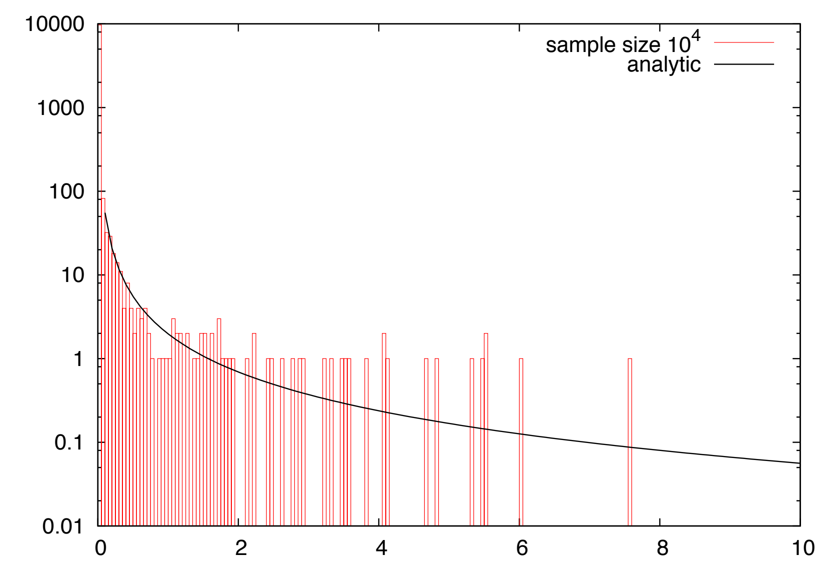
- Example: sample $\exp(-\frac{x^2}{2})$, reweight to $\exp(-\frac{(x-x_0)^2}{2}) \rightarrow \langle x \rangle = x_0$?



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



Insufficient overlap ($x_0 = 5$)



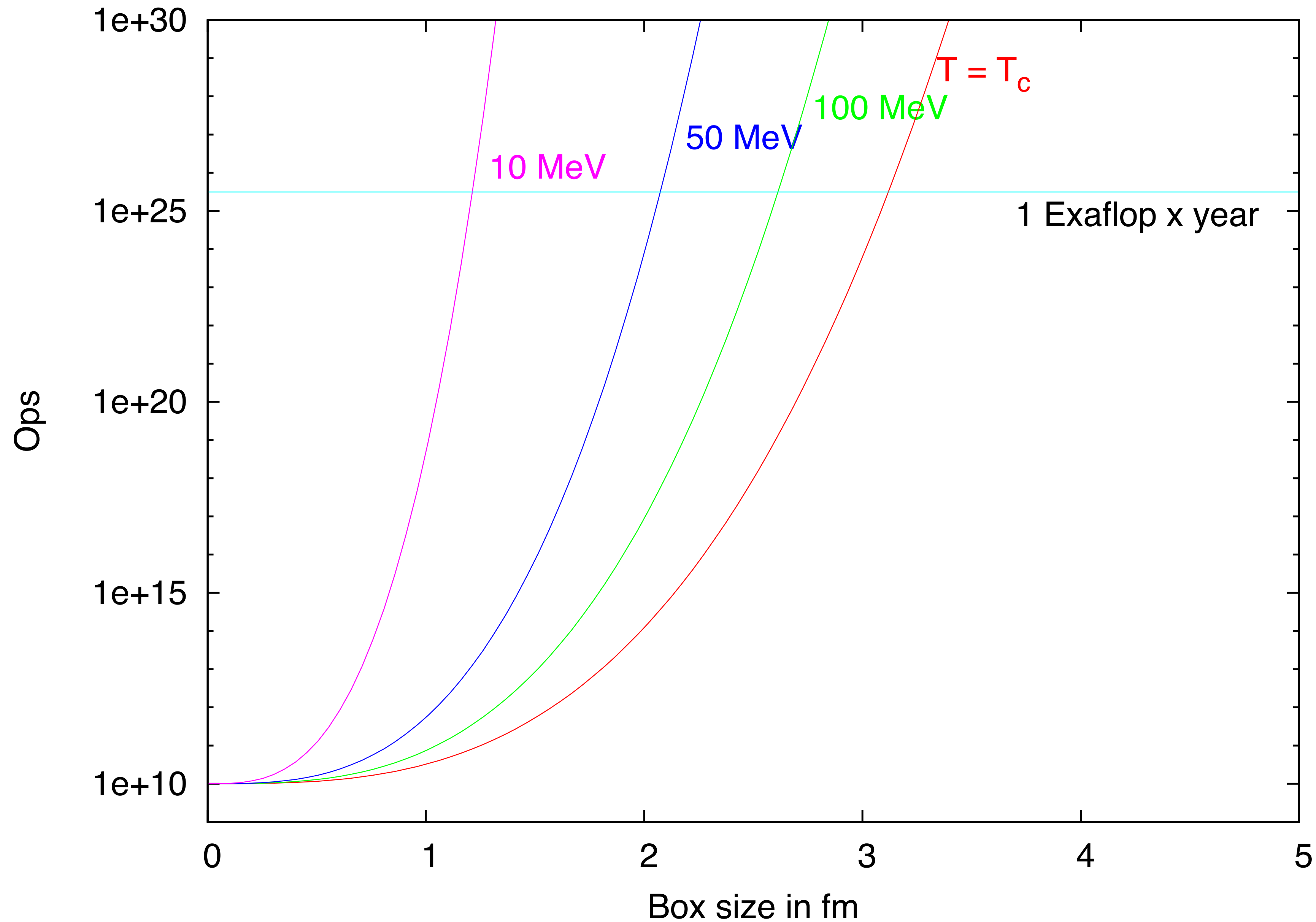
Very non-Gaussian distribution of reweighting factor

Log-normal Kaplan et al.

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

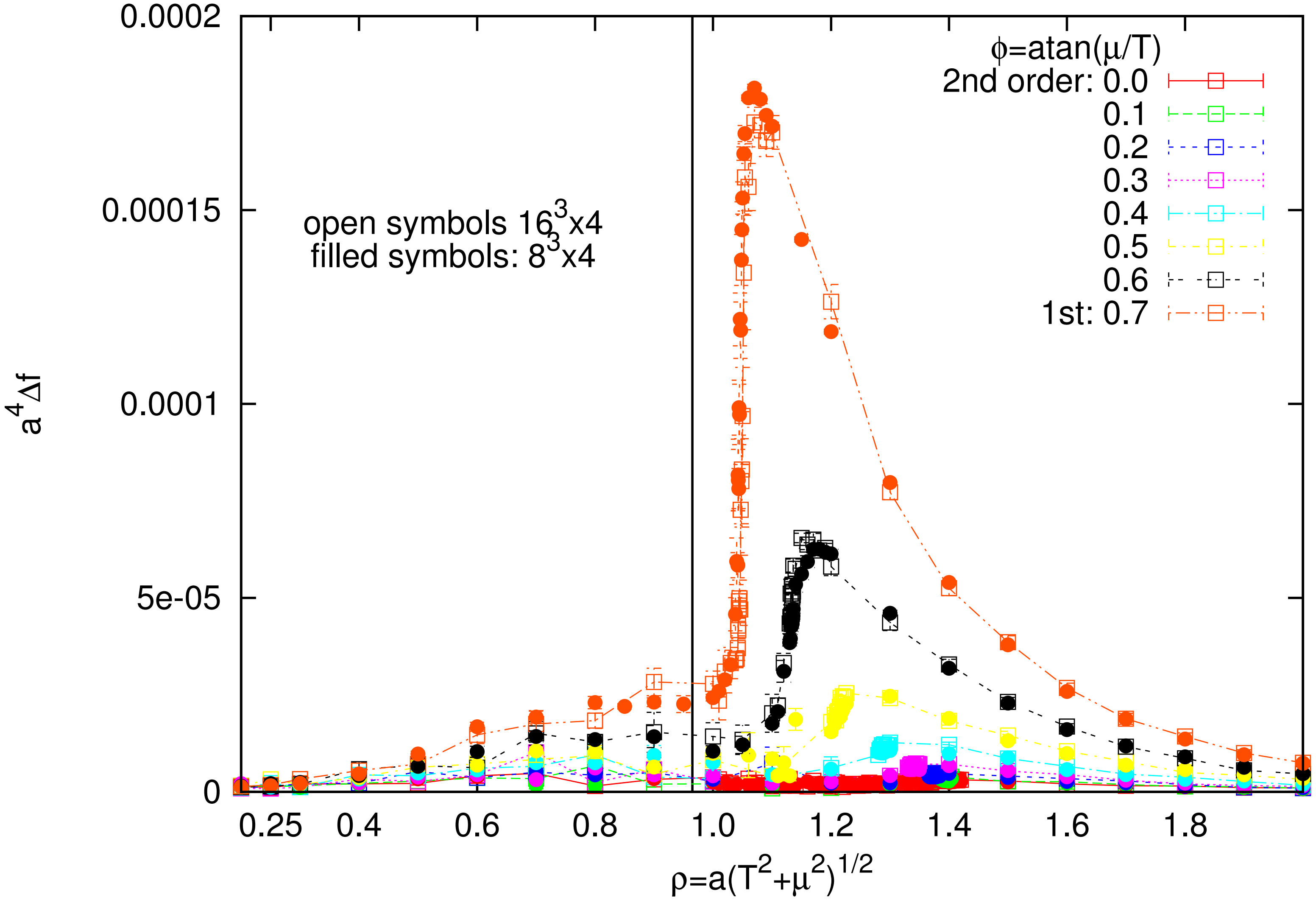
The CPU effort grows *exponentially* with L^3/T

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



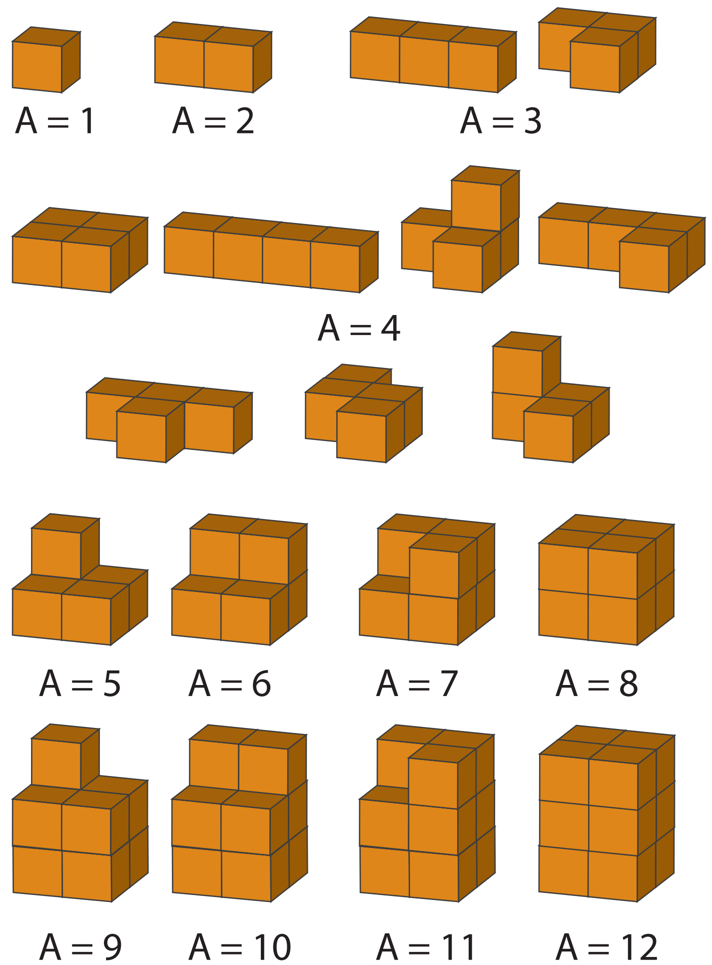
Crudely based on:
- 1 sec on 1GF laptop for 2^4 lattice, $a = 0.1$ fm
- effort $\propto \exp(2\frac{V}{T}\underbrace{\rho_{\text{nucl.}}(m_B - 3/2m_\pi)}_{\Delta f})$

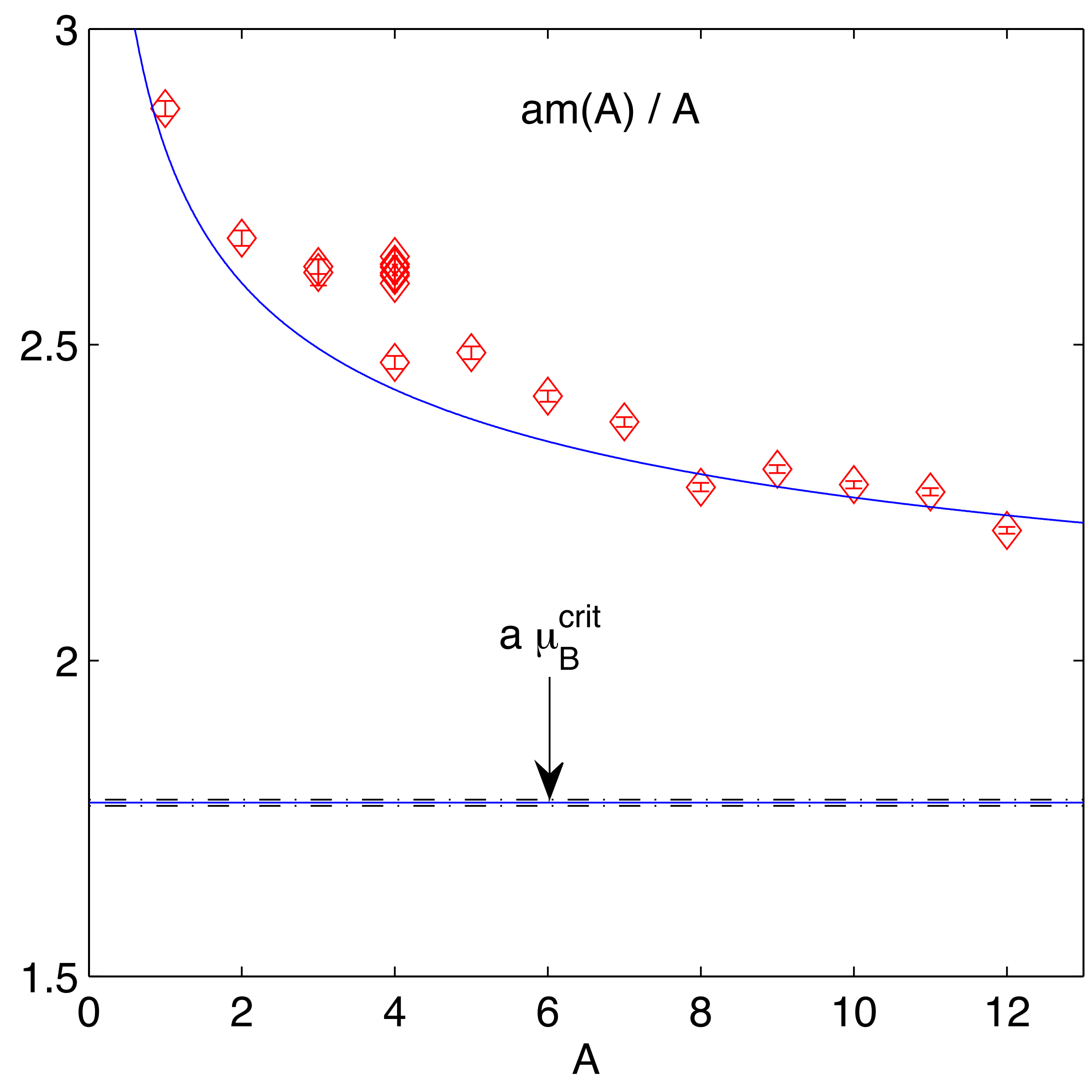
Severity of sign problem? Monitor $\Delta f = -\frac{1}{V} \log\langle \text{sign} \rangle$



- $\langle \text{sign} \rangle = \frac{Z}{Z_{||}} \sim \exp(-\frac{V}{T}\Delta f(\mu^2))$ 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 – Crude nuclear matter: spectroscopy w/Fromm





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

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